

Journal of Multiscale Modelling

Computational Homogenization of Heterogeneous Materials by a Novel Hybrid Numerical Scheme --Manuscript Draft--

Manuscript Number:	
Full Title:	Computational Homogenization of Heterogeneous Materials by a Novel Hybrid Numerical Scheme
Article Type:	Research Paper
Keywords:	Composite materials; Computational Micro-mechanics; Boundary Element Method; Virtual Element Method
Corresponding Author:	Ivano Benedetti, PhD Università degli Studi di Palermo Palermo, ITALY
Corresponding Author Secondary Information:	
Corresponding Author's Institution:	Università degli Studi di Palermo
Corresponding Author's Secondary Institution:	
First Author:	Marco Lo Cascio
First Author Secondary Information:	
Order of Authors:	Marco Lo Cascio Marco Grifò Alberto Milazzo, PhD Ivano Benedetti, PhD
Order of Authors Secondary Information:	
Abstract:	<p>The Virtual Element Method (VEM) is a recent numerical technique capable of dealing with very general polygonal and polyhedral mesh elements, including irregular or non-convex ones.</p> <p>Because of this feature, the VEM ensures noticeable simplification in the data preparation stage of the analysis, especially for problems whose analysis domain features complex geometries, as in the case of computational micro-mechanics problems.</p> <p>The Boundary Element Method (BEM) is a well-known, extensively used and effective numerical technique for the solution of several classes of problems in science and engineering.</p> <p>Due to its underlying formulation, the BEM allows reducing the dimensionality of the problem, resulting in substantial simplification of the pre-processing stage and in the reduction of the computational effort, without jeopardising the solution accuracy.</p> <p>In this contribution, we explore the possibility of a coupling VEM and BEM for computational homogenisation of heterogeneous materials with complex microstructures.</p> <p>The test morphologies consist of unit cells with irregularly shaped inclusions, representative e.g. of a fibre-reinforced polymer composite. The BEM is used to model the inclusions, while the VEM is used to model the surrounding matrix material. Benchmark finite element solutions are used to validate the analysis results.</p>
Suggested Reviewers:	Zahra Sharif-Khodaei, PhD Senior Lectures, Imperial College London z.sharif-khodaei@imperial.ac.uk She has worked with the Boundary Element Method and has expertise in computational modelling.
	Vincenzo Mallardo, PhD

Associate Professor, Università degli Studi di Ferrara
vincenzo.mallardo@unife.it
He has expertise in boundary element modelling and materials modelling

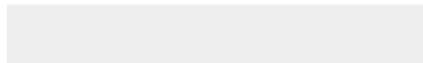
Vladislav Mantič
Full professor, Universidad de Sevilla Escuela Técnica Superior de Ingeniería de Sevilla
mantic@esi.us.es
He is an expert in boundary element methods and computational mechanics.



Click here to access/download

Supplemental File

2020_CoverLetter_LoCascioAL.pdf



Computational Homogenization of Heterogeneous Materials by a Novel Hybrid Numerical Scheme

Marco Lo Cascio,^{a)} Marco Grifò,^{b)} Alberto Milazzo,^{c)} and Ivano Benedetti^{d)}

Department of Engineering, University of Palermo, Viale delle Scienze, Edificio 8, 90128, Palermo, Italy

^{a)}Electronic mail: marco.locascio01@unipa.it

^{b)}Electronic mail: marco.grifo01@unipa.it

^{c)}Electronic mail: alberto.milazzo@unipa.it

^{d)}Corresponding author: ivano.benedetti@unipa.it

Abstract. The Virtual Element Method (VEM) is a recent numerical technique capable of dealing with very general polygonal and polyhedral mesh elements, including irregular or non-convex ones. Because of this feature, the VEM ensures noticeable simplification in the data preparation stage of the analysis, especially for problems whose analysis domain features complex geometries, as in the case of computational micro-mechanics problems. The Boundary Element Method (BEM) is a well-known, extensively used and effective numerical technique for the solution of several classes of problems in science and engineering. Due to its underlying formulation, the BEM allows reducing the dimensionality of the problem, resulting in substantial simplification of the pre-processing stage and in the reduction of the computational effort, without jeopardising the solution accuracy. In this contribution, we explore the possibility of a coupling VEM and BEM for computational homogenisation of heterogeneous materials with complex microstructures. The test morphologies consist of unit cells with irregularly shaped inclusions, representative e.g. of a fibre-reinforced polymer composite. The BEM is used to model the inclusions, while the VEM is used to model the surrounding matrix material. Benchmark finite element solutions are used to validate the analysis results.

INTRODUCTION

The Boundary Element Method (BEM) [1, 2] and the Finite Element Method (FEM) [3] are numerical techniques routinely employed for the solution of several classes of engineering and scientific problems. Both methods are widely used in solids and materials mechanics, where each of them has its own specific merits: while the FEM offers acknowledged generality and relative simplicity in including complex modelling aspects, such as domain inhomogeneity or non-linear material behaviours, the BEM is known to offer pre-processing simplification and high numerical accuracy at a relatively reduced computational cost, especially in problems requiring accurate representation of surfaces. For some classes of problems exhibiting regions with different properties, the consideration of such merits has suggested in the past the coupling the two methods in hybrid approaches combining their relative strengths [4].

The same considerations can be extended to the use of a recent generalisation of the FEM, known as the Virtual Element Method (VEM), [5] which presents some advantages with respect to the standard method. An important feature of the VEM is that it can handle very general polygonal and polyhedral mesh elements, including irregular or non-convex ones. For such a reason, the VEM provides appreciable simplification in the data preparation stage of the analysis, especially in problems whose analysis domain features complex geometries, e.g. in the case of computational micro-mechanics [6], which may induce irregular meshes when automatic algorithms are used. The BEM, on the other hand, has also been successfully employed for the computational homogenisation of materials with complex morphologies and multi-physics behaviour [7, 8, 9, 10, 11].

In this contribution, we explore the capabilities of a coupled VEM-BEM approach for computational homogenisation of heterogeneous materials with complex microstructures. This contribution is organised as follows. The Section *Formulation* briefly reviews the BEM and the lowest-order VEM for two-dimensional linear elastic problems and gives details of the adopted coupling procedure. The Section *Tests* presents the application of the hybrid procedure to a case study represented by a matrix with a complex shaped inclusion, assessing the accuracy in terms of displacements and stresses. Some concluding remarks are eventually given in the *Conclusions*.

FORMULATION

Let us consider a two-dimensional linear elastic problem set in the framework of small strains. The elastic body lies within the domain $\Omega \in \mathbb{R}^2$ with its external boundary $\Gamma = \partial\Omega$. It is assumed that no body forces act within Ω , but both tractions and/or displacements can be enforced on the boundary Γ . Without loss of generality, the domain Ω

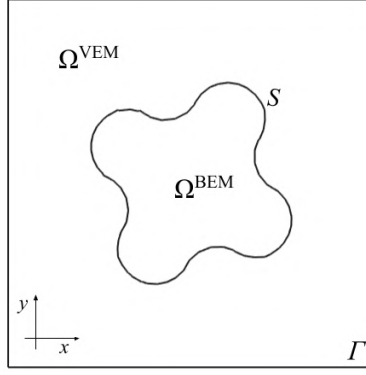


FIGURE 1: Model geometry: the BEM is employed to model the inclusion while the VEM models the surrounding medium.

is considered as the union of two subdomains, namely Ω^{BEM} and Ω^{VEM} that represent, respectively, an irregularly shaped inclusion, representative e.g. of the transversal section of a fibre in a polymer fibre-reinforced composite, and the surrounding matrix, representative e.g. of the polymer matrix in the mentioned class of materials. The two subdomains share the interface S , as shown in Fig. 1, where the considered analysis domain is drawn with its features.

In the proposed approach, the BEM is used to model the inclusion while the VEM is used to model the surrounding matrix. To this end, the domain Ω^{VEM} is partitioned into a number of polygons of general shape, while the boundary $S = \partial\Omega^{BEM}$ is divided into a number of segments, which form the edges of the polygonal elements in Ω^{VEM} lying in proximity of the interface between the two subdomains.

The boundary element formulation

For the BEM subdomain Ω^{BEM} with the smooth boundary $S = \partial\Omega^{BEM}$, in absence of body forces and using tensor notation with $i, j = x, y$, the boundary integral equation (BIE) for the displacements u_j at a boundary *collocation* point $\mathbf{x}_0 \in S$ can be written as [1]

$$\alpha_{ij}(\mathbf{x}_0) u_j(\mathbf{x}_0) = \int_S G_{ij}(\mathbf{x}_0, \mathbf{x}) t_j(\mathbf{x}) ds - \int_S H_{ij}(\mathbf{x}_0, \mathbf{x}) u_j(\mathbf{x}) ds \quad (1)$$

where the terms α_{ij} are functions of the geometry at the point \mathbf{x}_0 , $u_i(\mathbf{x})$ and $t_i(\mathbf{x})$ are unknown displacement and traction components at the *integration* boundary point \mathbf{x} . The fundamental solutions $H_{ij}(\mathbf{x}_0, \mathbf{x})$ and $G_{ij}(\mathbf{x}_0, \mathbf{x})$ for plane strain condition are given by

$$\begin{aligned} G_{ij}(\mathbf{x}_0, \mathbf{x}) &= C_1 (C_2 \delta_{ij} \ln r - r_{,i} r_{,j}) \\ H_{ij}(\mathbf{x}_0, \mathbf{x}) &= \frac{C_3}{r} [n_k r_{,k} (C_4 \delta_{ij} + 2r_{,i} r_{,j}) - C_4 (r_{,i} n_j - r_{,j} n_i)] \end{aligned} \quad (2)$$

where $r = |\mathbf{x} - \mathbf{x}_0|$ is the Euclidean distance between the points \mathbf{x}_0 and \mathbf{x} , the indicial notation $f_{,i} = \partial f / \partial x_i$ is adopted to refer to differentiation, n_i are components of the outward unit normal vector to the boundary S at the generic smooth point \mathbf{x} . The coefficients C_1 , C_2 , C_3 and C_4 are given by

$$C_1 = -\frac{1+\nu}{4\pi(1-\nu)E}, \quad C_2 = 3-4\nu, \quad C_3 = -\frac{1}{4\pi(1-\nu)}, \quad C_4 = 1-2\nu, \quad (3)$$

with E and ν denoting respectively the Young's modulus and the Poisson's ratio of the isotropic material within the subdomain Ω^{BEM} . It is worth noting that an analogous formulation can be adopted also for anisotropic inclusions, as long as the fundamental solutions are known.

The numerical solution of Eq.(1) is based on the discretisation of S and the subsequent approximation of the boundary displacement and traction components in terms of shape functions and nodal values. More specifically, S is subdivided into m straight segments ΔS_k and two nodes are associated with the extremes of each segment; each node

carries two components of displacements and two components of tractions. Since S is considered to be smooth, so that a tangent to it can be associated to any $\mathbf{x} \in S$, the existence of a unique value of traction at the node is ensured; in other words, corner points are not considered in the present formulation, although these could be treated resorting to known boundary element techniques [2].

We assume both displacement and traction components to be globally continuous over S and to vary linearly over each boundary segment ΔS_k according to

$$\mathbf{u}(\xi) = \mathbf{N}(\xi) \mathbf{u}^k, \quad \mathbf{t}(\xi) = \mathbf{N}(\xi) \mathbf{t}^k \quad (4)$$

where $\mathbf{N}(\xi) \in \mathbb{R}^{2 \times 4}$ is the matrix collecting 1D linear shape functions for the boundary segment ΔS_k , expressed as function of the natural coordinate ξ , and $\mathbf{u}^k, \mathbf{t}^k \in \mathbb{R}^{4 \times 1}$ collect, respectively, nodal components of displacements and tractions associated with the boundary segment ΔS_k .

Eq.(1), collocated at the generic boundary node p , may be rewritten in matrix notation as

$$\alpha \mathbf{u}_p = \sum_{q=1}^m \left[\int_{\Delta S_q} \mathbf{G}_{pq}(\xi) \mathbf{N}(\xi) J(\xi) d\xi \right] \mathbf{t}^q - \sum_{q=1}^m \left[\int_{\Delta S_q} \mathbf{H}_{pq}(\xi) \mathbf{N}(\xi) J(\xi) d\xi \right] \mathbf{u}^q \quad (5)$$

where $\alpha \in \mathbb{R}^{2 \times 2}$ is a matrix depending on the geometry of the boundary at the considered collocation point p , smooth in this case, $\mathbf{u}_p \in \mathbb{R}^{2 \times 1}$ collects the components of displacements at the node p , \mathbf{u}^q and \mathbf{t}^q are nodal displacements and tractions associated with ΔS_q , as in Eq.(4), and $J(\xi)$ indicates the absolute value of the Jacobian of the transformation between segment local and natural coordinates.

After integration and some algebraic manipulation, Eq.(5) may be rewritten in compact form as

$$\mathbf{H}_p \mathbf{U}^B = \mathbf{G}_p \mathbf{T}^B \quad (6)$$

where $\mathbf{H}_p, \mathbf{G}_p \in \mathbb{R}^{2 \times 2m}$ denote the rectangular matrices obtained by collocating at the node p and integration over the whole boundary S while $\mathbf{U}^B, \mathbf{T}^B \in \mathbb{R}^{2m \times 1}$ collect the components of displacements and tractions for all the nodes identified on the boundary S , with the superscript B introduced to highlight that such quantities are associated with the BEM domain. Writing Eq.(6) $\forall p \in [1, \dots, m]$, the subsequent set of linear algebraic equations

$$\mathbf{H} \mathbf{U}^B = \mathbf{G} \mathbf{T}^B \quad (7)$$

is obtained, where $\mathbf{H}, \mathbf{G} \in \mathbb{R}^{2m \times 2m}$ collect the coefficient obtained from the integration of Eq.(5) written for all the collocation points. It is worth noting that, when the BEM domain identifies an inclusion in the analysed domain, both \mathbf{U}^B and \mathbf{T}^B are unknown quantities that must be determined by interfacing Eq.(eq:BEMequation) with the equations obtained by the numerical model of the complementary matrix domain.

The virtual element formulation

In this section, we give a brief overview of the lowest-order VEM for linear two-dimensional elasto-static problems. In the proposed framework, such formulation is employed to model the domain Ω^{VEM} , which could be associated e.g. with the polymer matrix of a fibre reinforced composite material.

As mentioned above, the VEM can address general polygonal elements, including highly distorted or non-convex elements. In the case of the lowest order VEM, for a general polygonal element E , the element degrees of freedom are the values of the displacements components at each of its n vertex, which are collected into the vector \mathbf{u}_E . Analogously to what is done in standard FEM, it is assumed that the displacements field \mathbf{u} within the element is given by

$$\mathbf{u} = \mathbf{N}(\boldsymbol{\eta}) \mathbf{u}_E \quad (8)$$

where $\mathbf{N}(\boldsymbol{\eta})$ is the generic matrix containing the *virtual* shape functions $N_v(\boldsymbol{\eta})$ associated with each vertex v . Differently from standard FEM however, such shape functions are known only on the element edges of E , where they are globally continuous linear polynomials.

Since the shape functions $N_v(\boldsymbol{\eta})$ are not explicitly known within the polygonal element, from which their connotation as *virtual*, an explicit expression for the strains is not available. An approximated constant strain field $\boldsymbol{\varepsilon}^0$ is assumed within each element, which can be computed from the degrees of freedom \mathbf{u}_E as

$$\boldsymbol{\varepsilon}^0 = \boldsymbol{\Pi}_E \mathbf{u}_E \quad (9)$$

where $\mathbf{\Pi}_E \in \mathfrak{R}^{3 \times 2n}$ is the matrix representation of a projection operator defined as [12]

$$\mathbf{\Pi}_E = \frac{1}{A_E} \sum_{v=1}^n \int_{e_v} \mathbf{N}_v^E \mathbf{N}(\boldsymbol{\eta}) ds \quad (10)$$

where A_E is the area of the polygonal element E , bounded by its n edges e_v and

$$\mathbf{N}_v^E = \begin{bmatrix} n_x & 0 \\ 0 & n_y \\ n_y & n_x \end{bmatrix} \quad (11)$$

is the matrix containing the components n_x and n_y of the outward unit normal vector over each edge. The integrals appearing at the right-hand side of Eq.(10), which are carried out over the element edges, are exactly computable, since the restriction of the virtual shape functions N_v to such edges are piecewise linear polynomials.

The VEM elemental stiffness matrix \mathbf{K}_E is the sum of two terms

$$\mathbf{K}_E = \mathbf{K}_E^c + \mathbf{K}_E^s. \quad (12)$$

The first term is given by

$$\mathbf{K}_E^c = A_E \mathbf{\Pi}_E^T \mathbf{C} \mathbf{\Pi}_E, \quad (13)$$

where \mathbf{C} is represents the material stiffness tensor in Voigt notation. Moreover, since the approximate strains $\boldsymbol{\varepsilon}^0$ are assumed constant within the element, while the displacements \mathbf{u} are piecewise linear on the element edges, in general $\boldsymbol{\varepsilon}^0$ are not compatible with the nodal degrees of freedom \mathbf{u}_E . The computation of the discrete internal strain energy, using only the approximate constant strains $\boldsymbol{\varepsilon}^0$, may lead to zero-energy modes not associated with rigid body motion. For such a reason, a stabilisation strategy similar to that used in standard FEMs for elements with reduced integration is employed in the VEM and the stabilisation matrix \mathbf{K}_E^s appearing in Eq.(12) may be computed as e.g. in Ref. [13], which ensures the proper rank of the \mathbf{K}_E .

The equivalent nodal forces \mathbf{F}_E are computed as in the standard FEM from specified tractions $\bar{\mathbf{t}}$ over the element boundary $\partial E = \cup e_v$, i.e.

$$\mathbf{F}_E = \int_{\partial E} \mathbf{N}^T(\boldsymbol{\eta}) \bar{\mathbf{t}} ds. \quad (14)$$

Once the elemental matrices are built, the assembly of the VEM global matrices can be performed following standard FE procedures, to obtain the following sets of equations for the VEM subdomain

$$\mathbf{K}^V \mathbf{U}^V = \mathbf{F}^V \quad (15)$$

where \mathbf{K}^V , \mathbf{U}^V and \mathbf{F}^V are, respectively, the stiffness matrix, the nodal displacement vector and the force vector for the VEM subdomain, with the superscript V introduced to identify quantities related with the VEM domain.

Coupling procedure

The coupling of boundary and finite elements has been achieved in the literature using various approaches [4, 14, 15, 16, 17]. In this work, to couple the virtual and the boundary element methods, the BEM subdomain is treated as a macro-finite element and the *traction*-displacement equations associated with it are transformed into *force*-displacement equations and assembled with the VEM equations, already expressed in terms of nodal forces and displacements.

The vectors \mathbf{U}^V and \mathbf{F}^V appearing in Eq.(15) collect the displacement and nodal force components of all the VEM nodes in the considered domain. Since only some of such nodes belong to the interface \mathcal{S} , it is possible to partition the vectors as

$$\mathbf{U}^V = \begin{bmatrix} \mathbf{U}_S \\ \mathbf{U}_D \end{bmatrix}^V, \quad \mathbf{F}^V = \begin{bmatrix} \mathbf{F}_S \\ \mathbf{F}_D \end{bmatrix}^V, \quad (16)$$

where \mathbf{U}_S^V and \mathbf{F}_S^V identify components related to nodes belonging to S . Along S , the nodal displacements and forces must then satisfy the compatibility and equilibrium conditions

$$\mathbf{U}^B = \mathbf{U}_S^V, \quad \mathbf{F}^B + \mathbf{F}_S^V = \mathbf{0}, \quad (17)$$

which have been written considering that no external nodal forces act on the nodes belonging to S . The displacement compatibility equations can be readily written, as the same displacement components appear in both the BEM and VEM equations. On the contrary, while nodal forces appear in Eq.(15), related to the VEM domain, tractions appear in Eq.(7), related to the BEM domain, so that it is necessary to retrieve consistent nodal forces from BEM tractions, before writing the equilibrium equations appearing in Eq.(17).

This may be done, for a generic boundary element node, by resorting to appropriate energetic considerations. In the adopted scheme, since two-node piecewise linear boundary elements are used, a generic node always lies at the conjunction of two contiguous *boundary* elements. To avoid confusion, it is here recalled that, in the considered 2D background, boundary elements are 1D segments, which are then interfaced with the *edges* of the 2D virtual elements. If the generic node i lies between the boundary elements ΔS_k and ΔS_{k+1} , then, for a virtual displacement $\delta \mathbf{u}(\mathbf{x}_i) \equiv \delta \mathbf{u}_i$ of the node i , the unknown nodal force \mathbf{F}_i^B will perform a work that should be energetically equivalent to the work performed by the tractions acting on the two contiguous boundary elements. Thus, the following equivalence holds

$$\delta \mathbf{u}_i^T \mathbf{F}_i^B = \sum_{j=k}^{k+1} \int_{\Delta S_j} \delta \mathbf{u}^T(\xi) \mathbf{t}(\xi) J(\xi) d\xi, \quad (18)$$

which, recalling the interpolation expressed in Eq.(4), may be written as

$$\delta \mathbf{u}_i^T \mathbf{F}_i^B = \sum_{j=k}^{k+1} \delta \mathbf{u}^{j,T} \left[\int_{\Delta S_j} \mathbf{N}(\xi)^T \mathbf{N}(\xi) J(\xi) d\xi \right] \mathbf{t}^j = \sum_{j=k}^{k+1} \delta \mathbf{u}^{j,T} \mathbf{M}^j \mathbf{t}^j, \quad (19)$$

where $\mathbf{M}^j \in \mathbb{R}^{4 \times 4}$ stem from the integration over the considered elements of the shape functions matrices, while the vectors $\delta \mathbf{u}^j, \mathbf{t}^j \in \mathbb{R}^{4 \times 1}$ collect the components of displacements of the two end nodes belonging to the element j , so that

$$\delta \mathbf{u}^k = \begin{bmatrix} \delta \mathbf{u}_{i-1} \\ \delta \mathbf{u}_i \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \delta \mathbf{u}_i \end{bmatrix}, \quad \delta \mathbf{u}^{k+1} = \begin{bmatrix} \delta \mathbf{u}_i \\ \delta \mathbf{u}_{i+1} \end{bmatrix} = \begin{bmatrix} \delta \mathbf{u}_i \\ \mathbf{0} \end{bmatrix}. \quad (20)$$

Taking into account Eqs.(20), Eq.(19) may be rewritten

$$\delta \mathbf{u}_i^T \mathbf{F}_i^B = \delta \mathbf{u}_i^T \sum_{j=k}^{k+1} \tilde{\mathbf{M}}^j \mathbf{t}^j \quad \Rightarrow \quad \mathbf{F}_i^B = \sum_{j=k}^{k+1} \tilde{\mathbf{M}}^j \mathbf{t}^j \quad (21)$$

where $\tilde{\mathbf{M}}^j \in \mathbb{R}^{2 \times 4}$ is the sub-matrix extracted from \mathbf{M}^j selecting the appropriate rows corresponding to the displacements associated with the node i . It is important to realise that Eq.(21) allows expressing \mathbf{F}_i^B in terms of the traction components associated with the two elements containing the node i ; for two-node linear boundary elements such expression could be written as

$$\mathbf{F}_i^B = \sum_{k=i-1}^{i+1} \mathbf{M}_k \mathbf{t}_k \quad (22)$$

where \mathbf{t}_k collects the components of tractions of the node k . Once Eq.(22) is written for all the boundary element nodes belonging to S , the nodal forces \mathbf{F}^B appearing in the equilibrium equations, Eq.(17), can be expressed in terms of the boundary tractions \mathbf{T}^B appearing in Eq.(7) as

$$\mathbf{F}^B = \mathbf{M} \mathbf{T}^B, \quad (23)$$

where $\mathbf{F}^B, \mathbf{T}^B \in \mathbb{R}^{2m \times 1}$ and $\mathbf{M} \in \mathbb{R}^{2m \times 2m}$, with m expressing the total number of boundary nodes/elements.

Exploiting Eq.(23), Eq.(7) can be written in a form to be used in conjunction with the VEM equations; in particular, remembering that $\mathbf{T}^B = \mathbf{G}^{-1} \mathbf{H} \mathbf{U}^B$, it is possible to write

$$\mathbf{F}^B = \mathbf{M} \mathbf{T}^B = (\mathbf{M} \mathbf{G}^{-1} \mathbf{H}) \mathbf{U}^B = \mathbf{K}^B \mathbf{U}^B. \quad (24)$$

The above BEM equations can now be combined with the VEM equations, which can be rewritten as

$$\begin{bmatrix} \mathbf{K}_{SS} & \mathbf{K}_{SD} \\ \mathbf{K}_{DS} & \mathbf{K}_{DD} \end{bmatrix}^V \begin{bmatrix} \mathbf{U}_S \\ \mathbf{U}_D \end{bmatrix}^V = \begin{bmatrix} \mathbf{F}_S \\ \mathbf{F}_D \end{bmatrix}^V, \quad (25)$$

with the interface conditions in Eq.(17) and with suitable external boundary conditions to obtain the problem solution.

NUMERICAL TESTS

In this section, the proposed hybrid scheme is numerically assessed considering as test morphology a unit cell with an irregularly shaped inclusion, representative e.g. of a fibre-reinforced polymer composite. The BEM is used to model the inclusion, while the VEM is used to model the surrounding matrix material. The geometry of the unit cell is shown in Fig. 1. The materials of both the matrix and the inclusion are supposed isotropic and their Young's moduli are, respectively, $E_m = 5 \text{ GPa}$ and $E_f = 50 \text{ GPa}$, while the value of the Poisson's ratio for both materials is $\nu = 0.3$. Plane strain conditions are assumed and three sets of kinematic uniform boundary conditions are enforced on the unit cell. Such applied displacement boundary conditions correspond to a uniaxial macro-strain along the x -direction, a uniaxial macro-strain along the y -direction and a pure shear macro-strain acting to modify the angle between the axis x and y .

For benchmarking purposes, a pure FE mesh is created for both the matrix and the fibre, using linear triangular elements (TRIA3) Fig. 2a. A convergence study of the FE solution is performed, analysing four progressively refined meshes with $N_e = 2762, 7910, 12963, 19288$ TRIA3 elements respectively. The convergence is assessed by considering the convergence of the displacements of the nodes belonging to the interface S between the matrix and the inclusion. Fig. 3a shows no appreciable variation of the deformed interface with refined mesh sizes. Therefore, the FEM mesh with 2762 TRIA3 elements is chosen as benchmark. This FE model has 2898 degrees of freedom.

The VEM-BEM mesh (Fig. 2b) consists of $N_v = 1000$ 2D polygonal lowest-order VEM elements for the matrix domain and $N_b = 82$ 1D linear boundary elements for the interface between the inclusion and the matrix. The polygonal mesh exhibits 4016 degrees of freedom and was created using Polymesher [18], a mesh generator for polygonal elements written in MATLAB.

Fig. 3b shows the comparison between the deformed configuration of the interface obtained with the VEM-BEM and that previously obtained with the FEM as benchmark. For the same test case, Fig. 4 shows a comparison between the VEM-BEM model and the FEM model, in terms of deformed configuration and displacement magnitude, for the case of a uni-axial macro-strain along the x -direction. Eventually, Fig. 5 shows a comparison of the stress component σ_{xx} as obtained with the proposed strategy and with the benchmark FEM. Within the inclusion the stress components have been computed using their boundary integral representation. Analogous results in terms of accuracy were obtained for the all the considered test cases, which confirms that the proposed method could be profitably used for the micro-mechanical analysis of complex materials and for computational homogenization as well.

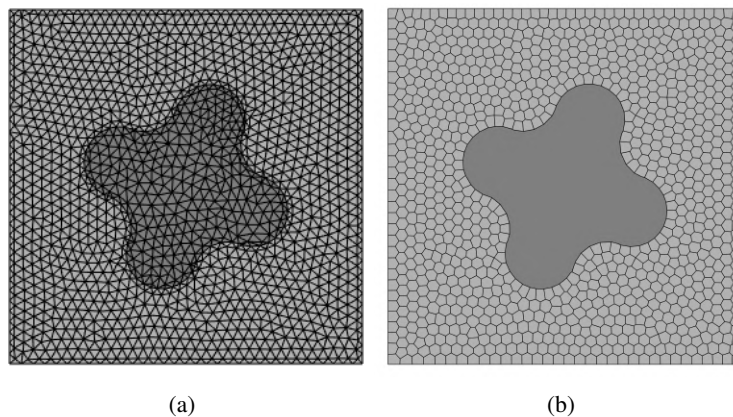


FIGURE 2: Mesh employed in (a) the pure FEs analysis and in (b) the VEM-BEM scheme .

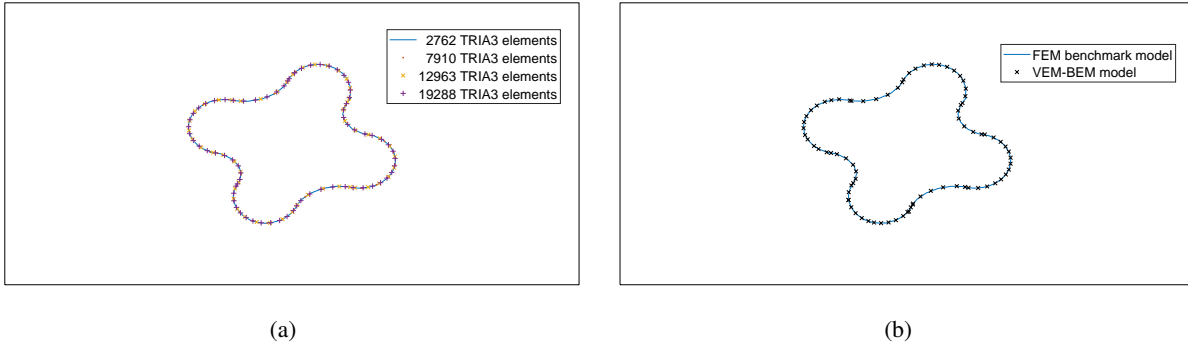


FIGURE 3: (a) FEM convergence analysis: the deformed interface is assessed at increasing mesh refinements; (b) Comparison of deformed interface of the VEM-BEM model against the FEM benchmark.

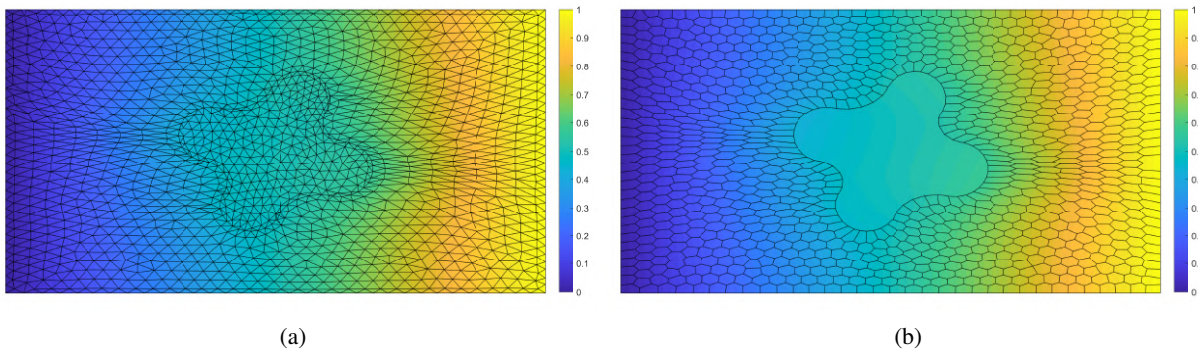


FIGURE 4: Deformed configuration with superimposed fringe plot of displacements for uniaxial macro-strain along the x direction: (a) FEM model; (b) VEM-BEM model.

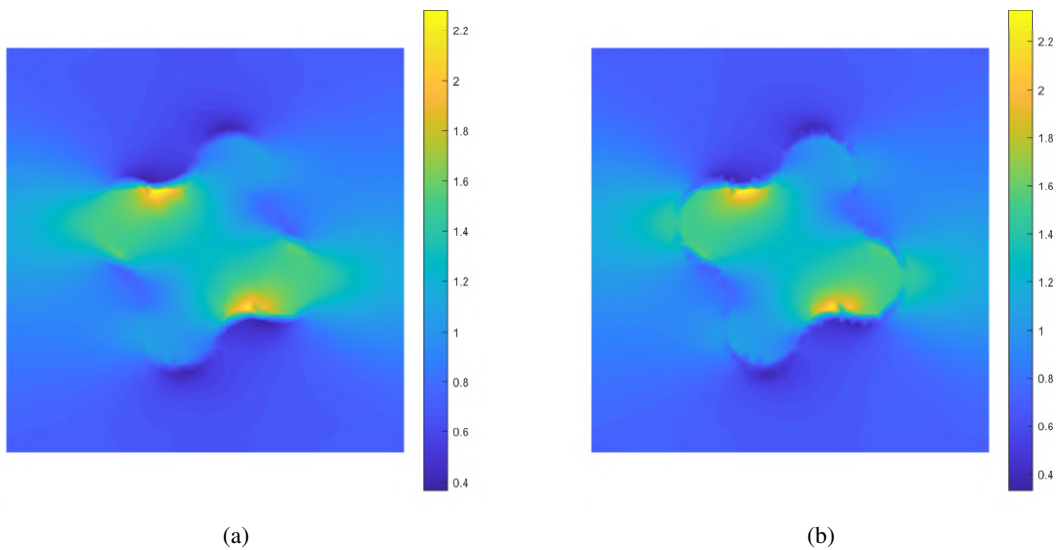


FIGURE 5: Stress component σ_{xx} for uniaxial macro-strain along the x direction: (a) FEM model; (b) VEM-BEM model. Values of stress are given in $\text{MPa} \times 10^4$.

ACKNOWLEDGMENTS

The authors acknowledge the support of the *Italian Ministry of Education, University and Research – MIUR* – through the project DEVISU, funded under the scheme PRIN-2107 – Grant 22017ZX9X4K_006.

CONCLUSIONS

A hybrid numerical formulation, based on the conjoined use of the virtual element method and the boundary element method, has been developed for the analysis of multi-region elastic problems involving complex morphologies, e.g. heterogeneous two-phase materials with inclusions of convoluted shape, which may be representative of fibre-reinforce polymer composites. The developed formulation has been implemented and tested on a case study and it has produced accurate results in terms of displacement and test fields. The results presented in this study provide an interesting preliminary step for the development of a flexible framework, suitable for the analysis of complex multi-phase material morphologies, thanks to the features of the VEM, which allow relaxing requirements on the mesh, and to the dimensionality reduction of the BEM. The systematic exploration of such potential benefit will form the object of further research.

REFERENCES

1. P. K. Banerjee and R. Butterfield, *Boundary element methods in engineering science*, Vol. 17 (McGraw-Hill London, 1981).
2. M. H. Aliabadi, *The boundary element method, volume 2: applications in solids and structures*, Vol. 2 (John Wiley & Sons, 2002).
3. O. C. Zienkiewicz, R. L. Taylor, P. Nithiarasu, and J. Zhu, *The finite element method*, Vol. 3 (McGraw-hill London, 1977).
4. C. Brebbia and P. Georgiou, "Combination of boundary and finite elements in elastostatics," *Applied Mathematical Modelling* **3**, 212–220 (1979).
5. L. Beirão da Veiga, F. Brezzi, A. Cangiani, G. Manzini, L. D. Marini, and A. Russo, "Basic principles of virtual element methods," *Mathematical Models and Methods in Applied Sciences* **23**, 199–214 (2013).
6. M. L. Cascio, A. Milazzo, and I. Benedetti, "Virtual element method for computational homogenization of composite and heterogeneous materials," *Composite Structures* **232**, 111523 (2020).
7. I. Benedetti and M. Aliabadi, "A three-dimensional grain boundary formulation for microstructural modeling of polycrystalline materials," *Computational Materials Science* **67**, 249 – 260 (2013).
8. V. Gulizzi, A. Milazzo, and I. Benedetti, "An enhanced grain-boundary framework for computational homogenization and micro-cracking simulations of polycrystalline materials," *Computational Mechanics* **56**, 631–651 (2015).
9. V. Gulizzi and I. Benedetti, "Micro-cracking of brittle polycrystalline materials with initial damage," *European Journal of Computational Mechanics* **25**, 38–53 (2016).
10. I. Benedetti, V. Gulizzi, and V. Mallardo, "A grain boundary formulation for crystal plasticity," *International Journal of Plasticity* **83**, 202 – 224 (2016).
11. I. Benedetti, V. Gulizzi, and A. Milazzo, "A microstructural model for homogenisation and cracking of piezoelectric polycrystals," *Computer Methods in Applied Mechanics and Engineering* **357**, 112595 (2019).
12. E. Artioli, L. B. Da Veiga, C. Lovadina, and E. Sacco, "Arbitrary order 2d virtual elements for polygonal meshes: part i, elastic problem," *Computational Mechanics* **60**, 355–377 (2017).
13. L. Beirão Da Veiga, F. Brezzi, and L. D. Marini, "Virtual elements for linear elasticity problems," *SIAM Journal on Numerical Analysis* **51**, 794–812 (2013).
14. O. Zienkiewicz, D. Kelly, and P. Bettess, "The coupling of the finite element method and boundary solution procedures," *International journal for numerical methods in engineering* **11**, 355–375 (1977).
15. L. Hong-Bao, H. Guo-Ming, H. A. Mang, and P. Torzicky, "A new method for the coupling of finite element and boundary element discretized subdomains of elastic bodies," *Computer Methods in Applied Mechanics and Engineering* **54**, 161–185 (1986).
16. T. Belytschko, H. Chang, and Y. Lu, "A variationally coupled finite element-boundary element method," *Computers & structures* **33**, 17–20 (1989).
17. T. Cruse and J. Osias, "Issues in merging the finite element and boundary integral equation methods," *Mathematical and Computer Modelling* **15**, 103–118 (1991).
18. C. Talischi, G. H. Paulino, A. Pereira, and I. F. Menezes, "Polymesh: a general-purpose mesh generator for polygonal elements written in matlab," *Structural and Multidisciplinary Optimization* **45**, 309–328 (2012).