Statistical Homogenization of Polycrystal Composite Materials with Thin Interfaces using Virtual Element Method

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Abstract

Polycrystalline materials with inter-granular phases are modern composite materials extremely relevant for a wide range of applications, including aerospace, defence and automotive engineering. Their complex microstructure is often characterized by stochastically disordered distributions, having a direct impact on the overall mechanical behaviour. In this context, within the framework of homogenization theories, we adopt a Fast Statistical Homogenization Procedure (FSHP), already developed in Pingaro et al. (2019), to reliably grasp the constitutive relations of equivalent homogeneous continua accounting for the presence of random internal structures. The approach, combined with the Virtual Element Method (VEM) used as a valuable tool to keep computational costs down, is here successfully extended to account for the peculiar microstructure of composites with polycrystals interconnected by thin interfaces. Numerical examples of cermet-like linear elastic composites complement the paper.

Keywords: Statistical Homogenization, Representative Volume Element, Random Composites, Grain Boundaries, Virtual Element Method

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1. Introduction

Modern composites materials are conceived to fulfil specific design requirements calling for the need of materials with increasingly high performances in terms of stiffness, strength, fracture toughness and lightness, among others. Special
5 attention has been devoted in the last decades to advanced ceramics, namely composites with ceramic (CMC) or metal matrix (MMC) [1, 2] which are gradually more used for a wide range of challenging applications, ranging from bio-engineering, with the production of biocompatible ceramics for prosthesis and artificial organs [3], aerospace, defence, automotive [4] up to mechanical en-
10 gineering for the production of wearing parts, seals, low weight components and fuel cells, and cutting tools with distinguished thermo-mechanical and wear properties [5]. Often ceramic composites exhibit a peculiar microstructure, characterized by polycrystals interconnected by a second-phase interphase of small thickness in comparison to the grain diameter. Consistently with [6], different
15 combinations of materials lead to four kinds polycrystalline materials with intergranular phases: i) ceramic grains with brittle interphases; ii) ceramic grains and a metallic interphase; iii) metallic grains surrounded by ceramic interphases; iv) metallic grains surrounded by a layer of soft ductile material. In all cases, such materials show complex phenonema occurring at different scales of inter-
20 est, ranging from the microscopic up to the macroscopic one, so that the elastic properties of the homogenized composite material is strongly influenced by the random distribution of grains, by the role played by the intergranular layer, as well as by the value of the contrast, that is defined as the ratio between the elastic moduli of the inclusions and the matrix [7, 8, 9].

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The reliable evaluation of homogenized constitutive properties to be adopted for the macroscopic investigation of their behaviour pertains to the well-established homogenization theories, and is a long-standing problem of great interest for many researchers [10, 11, 12, 13, 14, 15, 16], also with the purpose of designing
30 innovative smart materials [17, 18]. In this paper, we adopt a statistical ho-

mogenization approach [11, 19] to derive the in-plane linear elastic constitutive properties polycrystalline materials with thin layers interphases and to evaluate how they change in relation to contrast.

35 In the case of materials with random micro-structure, the lack of periodicity in the microscopic arrangement makes the homogenization process more challenging, asking for special attention in the detection of the Representative Volume Element (RVE) along with the evaluation of homogenized constitutive moduli. Several approaches have been proposed [20, 21, 22, 23, 24, 25, 26, 27, 14, 13, 40 28, 29], also referred to non-classical continua [30, 19, 9].

Among these models, we focus our attention on the possibility of approaching the RVE using finite-size scaling of intermediate control volume elements, named Statistical Volume Elements (SVEs), and proceed to homogenization (e.g. [31]). In this work we refer to [19], where a homogenization procedure 45 consistent with the Hill–Mandel condition [32] has been coupled with a statistical approach, by which scale-dependent bounds on classical moduli are obtained using Dirichlet and Neumann boundary conditions (BCs) for solving boundary value problems (BVPs). This statistically based homogenization procedure has provided significant results [30, 33, 34], with particular reference to the debated 50 problem of the convergence in the presence of materials with very low (or very high) contrast [9, 31, 25, 35].

More specifically, taking advantage of the encouraging results found in [36, 37], we here exploit an efficient evolution of the above mentioned procedure, i.e. the Fast Statistical Homogenization Procedure (FSHP) based on Virtual Ele- 55 ment Method (VEM). In FSHP the statistical procedure is automatized and integrated in a completely in house specifically developed code, that makes it possible to quickly and efficiently perform a high number of parametric analyses. VEM [38, 39] is an innovative and very promising computational method that find many engineering and structural mechanics applications [40, 41, 42, 60 41]: from linear [43, 44, 45] to non-linear elasticity [46, 47, 48], elastodynamic [49], topology optimization [50, 51], contact problem [52], plates [53], fracture

and damage [54, 55], as well as in homogenization of heterogeneous materials [56, 57, 36, 37].

Here, the procedure is to specifically account for the microstructural topology
65 exhibited by polycrystalline composites with thin interphases, making the most
of VEM to improve the computational efficiency. The result is a powerful numerical
tool suitable for analyses of large portions of random microstructure, very
important in the case materials with very high or low contrast [37]. In particular
the strategy proposed is to use a single virtual element for each grain (polygons
70 of any shape with n -nodes) with a significant reduction of the computational
burden, while the interconnecting layer is discretized with a fine mesh of triangular
elements. Other advantages of VEM are: capability of using hanging
nodes, that permits local refinements and coupling different degree elements;
robustness to distortion of the elements; perfectly coupling with FEM elements;
75 accuracy because the stiffness matrix is computed in precision machine; easy
implementation.

In this paper, low order virtual elements are used: the adoption of virtual
elements of order one is particularly suitable for the homogenization procedure,
as shown in [36, 37, 58]. Moreover, stress/strain is constant over the elements,
80 but this approximation does not affect homogenization results. Furthermore, by
the adoption of the hanging nodes we subdivide the edges of the grains for
generating a sufficiently fine mesh in the interphase part.

Exploiting FSHP combined with VEM, several parametric analyses have been performed
to characterize overall mechanical parameters of polycrystalline composites
85 with thin interphase layers and to investigate their sensitivity to the contrast
[59, 60]. Attention is paid both at the identification of the RVE size and at the
evaluation of the overall mechanical properties, that vary in relation with the
contrast of the material.

The outline of the paper is as follows. In Section 2 the statistical procedure
90 is recalled and specialized to the case at hand of polycrystals with thin inter-
granular layers. Section 3 is devoted to the basic assumption of the first order
virtual element formulation. Section 4 provides results of a set of parametric

analyses on cermet-like polycrystals with intergranular phases stiffer or softer than grains. In order to check the capabilities of the proposed procedure, a
95 successful comparison between the results obtained with VEM and those with a very fine FEM mesh is performed. In Section 5 some final remarks are presented, highlighting the expected advantages of the proposed approach with respect to more standard approaches.

2. Fast Statistical Homogenization Procedure

100 The main features of the so-called Fast Statistical Homogenization Procedure (FSHP), developed by the authors in [36, 37], are detailed in this Section. First, the attention is focused on two types of composites, characterized either by circular inclusions embedded in a base matrix or by polycrystalline material with thin interfaces, for which a linear elastic constitutive behaviour is assumed
105 at both the microscopic and the macroscopic level. Then, the key ideas of the statistical homogenization procedure are briefly recalled and specialized for the materials at hand.

2.1. Computational homogenization

We take into account a two-dimensional continuum and describe, at the microscopic scale, the heterogeneous composite as a two-phase material. We
110 both investigate the case of composites made of circular inclusions of diameter d , randomly distributed in a matrix (Fig. 1(a)), and the case of polycrystals (considered as inclusions) bounded by thin interfaces with average dimension $\bar{d}$ (Fig. 1(b)). The former case is representative of ceramic/metal matrix composites or also concrete or rocks, while the latter one is representative of cermets.
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In the present instance of non periodic composite materials and in view of the statistical homogenization procedure, it is useful to introduce a scale parameter $\delta = L/d^*$ defined as the ratio between the edge of a square test window L , and
120 the characteristic dimension d^* . We furthermore define the material contrast as the ratio between the elastic moduli of inclusions, E_i , and matrix, E_m , $c = E_i/E_m$. When $0 < c < 1$ ($c = 1$ being the case of a homogeneous material), inclusions are softer than the matrix and we refer to this case as *low contrast materials*, that are suitable to properly represent porous media [61]. On the
125 other hand, when $c > 1$ inclusions are stiffer than the matrix and we refer to *high contrast materials* [19].

In order to perform homogenization, we describe the material at two scales of interest: the microscopic and the macroscopic levels. At the microscopic level the

(a) Two-phases material with circular inclusions

(b) Polycrystal material with thin interfaces

Figure 1: Portions of heterogeneous material. The matrix and inclusions are depicted in red and blue, respectively.

heterogeneous material is represented in detail, accounting for each constituent in terms of geometry and constitutive behaviour. At the macroscopic level the composite material is ideally replaced by an equivalent material whose global behaviour is representative of the actual heterogeneous material. The governing equations are formally the same as those defined at the microscopic level, except for the constitutive law that is not ‘a priori’ defined at the macroscopic level, but directly descends from the lower level as result of the homogenization procedure. In the following, lower case letters always refer to the micro-scale, while upper case letters to the macro-scale.

We refer to a linearised two-dimensional framework. At the lower level each material phase is characterized by linear elastic isotropic behaviour with the

stress-strain relations written as:

$$\sigma_{ij} = \lambda \varepsilon_{kk} \delta_{ij} + 2\mu \varepsilon_{ij} , \quad (1)$$

where ε_{ij} and σ_{ij} ($i, j, k = 1, 2$) are the components of the micro-strain and micro-stress tensors, λ and μ are the Lamé constants, and δ_{ij} ($i, j = 1, 2$) is the Kronecker symbol. At the macroscopic level, the general anisotropic stress-strain relations, read:

$$\Sigma_{ij} = \mathbb{C}_{ijhk} E_{hk} , \quad (2)$$

where E_{ij} , Σ_{ij} ($i, j = 1, 2$) are the components of the macro-strain and macro-stress tensors and $\mathbb{C}_{ijhk}$ ($i, j, h, k = 1, 2$) are the homogenized moduli, i.e the components of the macroscopic elastic tensor obtained via a homogenization procedure based on the Hill's macro-homogeneity condition [32]:

$$\Sigma_{ij} E_{ij} = \frac{1}{A_\delta} \int_{\mathcal{B}_\delta} \sigma_{ij} \varepsilon_{ij} dA , \quad (3)$$

which states an energy equivalence between the macroscopic point and the corresponding domain (test window), $\mathcal{B}_\delta$, occupying a region of area A_δ at the microscopic level.

The homogenization procedure is based on the solution of properly defined boundary value problems at the microscopic level with Dirichlet and Neumann boundary conditions on the boundary $\partial\mathcal{B}_\delta$, directly deriving from the fulfilment of the macro-homogeneity condition, Eq. (3). The Dirichlet and Neumann BCs reads, respectively:

$$\underbrace{u_i = E_{ij} x_j, \text{ on } \partial\mathcal{B}_\delta}_{\text{Dirichlet BCs}}, \quad \underbrace{t_i = \Sigma_{ij} n_j, \text{ on } \partial\mathcal{B}_\delta}_{\text{Neumann BCs}}, \quad (4)$$

130 u_i being the components of the displacement vector and x_j ($i, j = 1, 2$) the coordinates of the generic point on the boundary, $\partial\mathcal{B}_\delta$, with respect to a reference system with origin in the geometric center of the test window $\mathcal{B}_\delta$. t_i are the components of the traction vector and n_j the component of the outward normal to $\partial\mathcal{B}_\delta$ ($i, j = 1, 2$).

135 2.2. Statistical Homogenization

FSHP is based on the statistical homogenization procedure previously developed in [19] and briefly described in Section 1. The proposed homogenization procedure is conceived for evaluating both the homogenized elastic parameters of a non-periodic heterogeneous material and for identify the Representative
140 Volume Element (RVE), that in the absence of a repetitive micro-structure is not known a priori.

According to the approach presented in [19], as well as in [21, 11], the presented procedure requires the statistical definition of a number of realizations called Statistical Volume Elements (SVEs), representing the micro-structure,
145 sampled in a Monte Carlo sense, which allows for determining series of scale-dependent upper and lower bounds for the overall elastic moduli and to approach the RVE size, δ_{RVE} , using a statistical stopping criterion, which is based on the variation of the average elastic moduli.

All steps of the homogenization procedure are completely integrated in the
150 FSHP and they are described below.

Step 1 Input: in the case of disk-shaped inclusion, we set set the nominal volume fraction of the medium ($\rho \leq 40\%$) as $\sum_{k=1}^{n_i} A_k/L^2$ in which A_k and L^2 are the area of k -th inclusion and area of a test window, respectively. If the particles are disk-shaped inclusions, with diameter d , randomly
155 distributed on the base of a planar ‘hard-core’ Poisson point field with distance, s , between the particles, fixed in order to avoid very narrow necks between inclusions. Define the dimensionless scale factor $\delta = L/d$. In the case of polycrystalline materials with thin interfaces, we set the average dimension of the grains $\bar{d}$ and define the dimensionless scale factor
160 $\delta = L/\bar{d}$. The parameter s is the thickness of the layer around the grains and in this work it is assumed constant for all grains boundaries.

Fix the mechanical parameters of each phase: Young modulus of inclusions and matrix, E_i and E_m ; Poisson coefficient, ν_i and ν_m . Set the minimum number of simulations for convergence, N^{lim} , and a tolerance parameter,

165 Tol , based on data dispersion, as defined in above.

Step 2 Input: initialize the window size, $L = L_0$, and number of simulations,
 $N = N_0$.

Step 3 Realizations: for the case of circular inclusion the procedure automati-
 cally determine for each window size the number of inclusions (Poisson
 170 random variable) via simulations exploit Knuth's algorithm (see [59, 36]).
 Then simulate random dispositions of disks' centers, according to the uni-
 form distribution, that are the realizations (SVEs) of portions of the ran-
 dom medium. Otherwise, the procedure generate a random polygonal
 mesh with average dimension of grains $\bar{d}$ calling the **Matlab**[®] program
 175 **PolyMesher** developed by [62]. Then all edges are shifted inwards by $s/2$
 in order to obtain the final geometry of all realizations $\mathcal{B}_\delta$. In Fig. 2 a
 schematic of the procedure is depicted for a generic grain: the initial poly-
 gon has vertices P_i ; additional points $\hat{P}_i$ are identified as a result of the
 shifting procedure, so that the interface area (in light blue) and the grain
 area (in light red) are defined.

Figure 2: Example of shift procedure starting by initial polygonal mesh obtained by
PolyMesher [62]

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In all cases, each realization is supposed to be independent from any previ-

Figure 3: Example of realization obtained by FSHP for different window size L

ous one. An examples of realization of the micro-structure and the related generated mesh for circular and polycrystal inclusions are shown in Figs. 1(a)-1(b). In Fig. 3 a realization obtained by FSHP for different windows size has been plotted.

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Step 4 Generate/Solve: for each SVE, generate the relative mesh and solve both the Dirichlet and Neumann (Eq. (4)) BVP, and compute the homogenized

constitutive parameters.

Step 5 Compute: evaluate the average bulk modulus, $\langle \mathbb{K} \rangle_\delta$, the relative standard deviation $\sigma(\langle \mathbb{K} \rangle_\delta)$ and variation coefficient $CV(\langle \mathbb{K} \rangle_\delta)$. Then compute $N_i = (1.96 \sigma(\langle \mathbb{K} \rangle_\delta) / (\langle \mathbb{K} \rangle_\delta Tol)^2$, which ensures that the confidence interval of the average homogenized constitutive parameter set at 95%, evaluated over the normal standard distribution, is within the tolerance allowed, Tol . Repeat Steps 3-4 until $N_i < N^{lim}$.

Step 6 Checking: if the number of realizations necessary for ensuring the requirement at Step 5 is small enough, stop the procedure. We choose as the number of realizations necessary the most unfavourable number between those obtained by solving BVPs of Neumann or Dirichlet. Otherwise choose an increased value of δ and go to Step 3.

The whole procedure has been schematized in the flow-chart in Fig. 4.

The fulfilment of the requirement at Step 6 means that the values of the homogenized constitutive coefficients are distributed around their averages with a vanishing variation coefficient, and that the RVE size is achieved. The effective homogenized elastic moduli can be determined as the mean value between the Dirichlet (upper) and Neumann (lower) bounds at the convergence window (RVE).

The statistical convergence criterion adopted is based on a 95% confidence level of the Normal Standard distribution, which provides the number N of realizations at which is possible to stop the simulations for a given window size δ .

When this number is small enough, the average values of the effective moduli converge and the RVE size is achieved. This circumstance also corresponds to reaching the minimum window size δ_{RVE} for which the estimated homogenized moduli remain constant, within a tolerance interval less than 0.5% for both the Dirichlet and Neumann solutions. The minimum number of simulations, N^{lim} , and the tolerance parameter, Tol , are chosen in order to define a narrow confidence interval for the average and to obtain a reliable convergence criterion. The adopted statistical criterion allows us to detect the RVE size also when the

Dirichlet and Neumann solutions do not tend to the same value. The values of the tolerance are assumed as a function of the data dispersion [19].

220 For all realizations of the micro-structure the Virtual Element Method (VEM) has been adopted as a numeric tool, that permits to adopt single polygonal element for the inclusions without meshing with consequently high reduction of the computational burden with respect to finite elements. Moreover, the adoption of the VEM allows us to create a refined mesh in the interface without
225 meshing the granular elements thanks to the use of so-called hanging nodes (Fig. 5). In the zones of interfaces a triangular virtual element mesh have been adopted, determined using a code for generating random mesh of Delaunay type (`Triangle`, [63]). As demonstrated in [64], three nodes virtual elements behaves just like 3-noded triangular finite elements.

230 The computational strategies adopted are aimed at making the statistical homogenization process as efficient as possible. This allow us to fast solve series (hundreds) of BVPs and to rapidly converge to the RVE solution.

Figure 4: Flow-chart of the Fast Statistical Homogenization Procedure

Figure 5: Example of the mesh in the interface zone between the grains obtained using the procedure

3. Virtual Element Framework

In this section we briefly recall the governing equation of the linear elastostatic problem and the related weak formulation, mandatory starting point to describe the construction of virtual element. We restrict our investigation to virtual elements of degree 1 [38, 39] also referred as lower order virtual elements. The Voigt notation is adopted since is more suited to easily develop the VEM formulation.

3.0.1. The linear elastic problem

We consider a two-dimensional domain, Ω , with Γ being its boundary. The body is subjected to the volume force, represented by the vector $\mathbf{f} \in (L^2(\Omega))^2$, $\mathbf{f} = \{f_1, f_2\}^T$ (within the standard Lebesgue space), and given boundary conditions, under the hypothesis of small deformations. For the sake of simplicity, we consider homogeneous Dirichlet boundary conditions to define the deformation problem of a linear elastic continuum. We introduce the Sobolev space, $\mathbf{V} := (H_0^1(\Omega))^2$, of the admissible displacement fields, represented by the vector $\mathbf{v}$. Furthermore we represent the strain as the vector $\boldsymbol{\varepsilon}(\mathbf{u})$ associated to the displacement field vector $\mathbf{u} = \{u_1, u_2\}^T$:

$$\boldsymbol{\varepsilon}(\mathbf{u}) = \{\varepsilon_{11}, \varepsilon_{22}, 2\varepsilon_{12}\}^T = \{\partial_x u_1, \partial_y u_2, \partial_y u_1 + \partial_x u_2\}^T, \quad (5)$$

where $\partial_{(\cdot)}$ denotes the partial derivative with respect to the $(\cdot)$ -coordinate.

The weak form of the linear elastostatic problem, provided by the virtual work principle, reads:

$$\left\{ \begin{array}{l} \text{Find } \mathbf{u} \in \mathbf{V} \text{ such that :} \\ a(\mathbf{u}, \mathbf{v}) = \mathcal{F}(\mathbf{v}) \quad \forall \mathbf{v} \in \mathbf{V} \end{array} \right. \quad (6)$$

where the continuous bilinear form $a(\cdot, \cdot) : \mathbf{V} \times \mathbf{V} \rightarrow \mathbb{R}$, in witch $\mathbb{R}$ is the set of the real numbers, reads:

$$a(\mathbf{u}, \mathbf{v}) = \int_{\Omega} \boldsymbol{\varepsilon}(\mathbf{v})^T \mathbb{C} \boldsymbol{\varepsilon}(\mathbf{u}) d\Omega, \quad (7)$$

in witch $\mathbb{C}$ is the 3×3 elastic tensor, and the linear functional $\mathcal{F}(\cdot) : \mathbf{V} \rightarrow \mathbb{R}$, reads:

$$\mathcal{F}(\mathbf{v}) = \int_{\Omega} \mathbf{f}^T \mathbf{v} d\Omega . \quad (8)$$

3.0.2. Virtual element formulation

In this subsection we introduce the virtual element discretization used in the homogenization procedure. In order to approximate the solution of the problem (6) we consider a decomposition $\mathcal{T}_h$ of the domain Ω into non overlapping polygonal elements E . In the following, we denote by e the straight edges of the mesh $\mathcal{T}_h$ and, for all $e \in \partial E$, $\mathbf{n}_i$ denotes the outward unit normal vector to e_i (Fig. 6(a)). The symbol n_e represents the number of the edges of the polygon E .

Let k be an integer ≥ 1 . Let us denote by $\mathcal{P}_k(\Omega)$ the space of polynomials, living on the set $\Omega \subseteq \mathbb{R}^2$, of degree less than or equal to k .

By the discretization introduced, it is possible to write the bilinear form (6), as in the finite element methodology, in the following way:

$$a(\mathbf{u}, \mathbf{v}) = \sum_{E \in \mathcal{T}_h} a^E(\mathbf{u}, \mathbf{v}) \quad \forall \mathbf{v} \in \mathbf{V} . \quad (9)$$

The discrete virtual element space, $\mathbf{V}_h$, is:

$$\mathbf{V}_h := \{ \mathbf{v} \in \mathbf{V} : \mathbf{v}|_E \in \mathbf{V}_{h|E} \forall E \in \mathcal{T}_h \} , \quad (10)$$

where the local space, $\mathbf{V}_{h|E} := [V_{h|E}]^2$. For the virtual element of degree $k = 1$, $V_{h|E}$ is defined as:

$$V_{h|E} := \{ \mathbf{v}_h \in H^1(E) \cap C^0(E) : \Delta \mathbf{v}_h \in \{0\}, \mathbf{v}_h|_e \in \mathcal{P}_1(e) \forall e \in \partial E \} . \quad (11)$$

The dimension of the space $\mathbf{V}_{h|E}$ then is:

$$m = \dim(\mathbf{V}_{h|E}) = 2n_e . \quad (12)$$

We can observe that, in contrast to the standard finite element approach, the local space $\mathbf{V}_{h|E}$ is not fully explicit. Moreover $\mathbf{v}_h$ is a polynomial of degree 1 on each edge e of E and globally continuous on ∂E .

(a)

(b)

Figure 6: Example of virtual element, E , with the relative nodes and edges numeration (a) and degrees of freedom of the virtual element of degree 1 (b).

The problem (6) restricted to the discrete space $\mathbf{V}_h$ becomes:

$$\left\{ \begin{array}{l} \text{Find } \mathbf{u}_h \in \mathbf{V}_h \text{ such that} \\ a_h(\mathbf{u}_h, \mathbf{v}_h) = \mathcal{F}(\mathbf{v}_h) \quad \forall \mathbf{v}_h \in \mathbf{V}_h, \end{array} \right. \quad (13)$$

where $a_h(\cdot, \cdot) : \mathbf{V}_h \times \mathbf{V}_h \rightarrow \mathbb{R}$ is the discrete bilinear form approximating the continuous form $a(\cdot, \cdot)$ and, $\mathcal{F}(\mathbf{v}_h)$ is the term approximating the virtual work of external load. In this work the body force is null, so no details for its imple-

mentation are reported. The discrete bilinear form is constructed element by element as

$$a_h(\mathbf{u}_h, \mathbf{v}_h) = \sum_{E \in \mathcal{T}_h} a_h^E(\mathbf{u}_h, \mathbf{v}_h) \quad \forall \mathbf{u}_h, \mathbf{v}_h \in \mathbf{V}_h, \quad (14)$$

265 By the above definition of the local space (11), the following important observations can be made:

- the functions $\mathbf{v}_h \in \mathbf{V}_{h|E}$ are explicitly known on ∂E (linear functions);
- the functions $\mathbf{v}_h \in \mathbf{V}_{h|E}$ are not explicitly known inside the element E ;
- $(\mathcal{P}_1(E))^2 \subseteq \mathbf{V}_{h|E}$.

270 The related degrees of freedom for the space $\mathbf{V}_{h|E}$ are $2n_e$ point-wise values $\mathbf{v}_h(v_i)$ $i = 1, 2, \dots, n_e$, where v_i is the i -th corner of E .

3.0.3. Projection operator and construction of the stiffness matrix

In accordance to [65] we define the projector operator of the strain as:

$$\begin{aligned} \Pi : \mathbf{V}_{h|E} &\rightarrow \mathcal{P}_0(E)_{sym}^{2 \times 2} \\ \mathbf{v}_h &\rightarrow \Pi(\mathbf{v}_h) \end{aligned} \quad (15)$$

More specifically, the projector operator respects the following orthogonality condition:

$$\int_E \Pi(\mathbf{v}_h)^T \hat{\boldsymbol{\varepsilon}} dE = \int_E \boldsymbol{\varepsilon}(\mathbf{v}_h)^T \hat{\boldsymbol{\varepsilon}} dE \quad \forall \hat{\boldsymbol{\varepsilon}} \in \mathcal{P}_0(E)_{sym}^{2 \times 2}. \quad (16)$$

As in the finite element method, we define the vectors $\mathbf{v}_h \in \mathbf{V}_{h|E}$ and $\hat{\boldsymbol{\varepsilon}} \in \mathcal{P}_0(E)_{sym}^{2 \times 2}$ using the degrees of freedom $\bar{\mathbf{v}}_h \in \mathbb{R}^{2n_e}$, $\bar{\boldsymbol{\varepsilon}} \in \mathbb{R}^3$:

$$\begin{cases} \mathbf{v}_h = \mathbf{N}^V \bar{\mathbf{v}}_h, \\ \hat{\boldsymbol{\varepsilon}} = \mathbf{N}^u \bar{\boldsymbol{\varepsilon}}. \end{cases} \quad (17)$$

The matrices $\mathbf{N}^u$ and $\mathbf{N}^V$ are

$$\mathbf{N}^u = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \mathbf{N}^V = \begin{bmatrix} \phi_1 & 0 & \cdots & \phi_{n_e} & 0 \\ 0 & \phi_1 & \cdots & 0 & \phi_{n_e} \end{bmatrix}, \quad (18)$$

where ϕ_i is the standard i -th shape function. The projection operator in matrix is:

$$\Pi(\mathbf{v}_h) = \mathbf{N}^u \bar{\Pi} \bar{\mathbf{v}}_h, \quad (19)$$

with $\bar{\Pi} \in \mathbb{R}^{3 \times m}$.

By putting Eqs. (17), (19) into the Eq. (16) we obtain:

$$\int_E (\mathbf{N}^u \bar{\Pi} \bar{\mathbf{v}}_h)^T \mathbf{N}^u \bar{\boldsymbol{\varepsilon}} dE = \int_E [\boldsymbol{\varepsilon} (\mathbf{N}^V \bar{\mathbf{v}}_h)]^T \mathbf{N}^u \bar{\boldsymbol{\varepsilon}} dE \quad \forall \bar{\boldsymbol{\varepsilon}} \in \mathbb{R}^3. \quad (20)$$

Integrating by part the right hand side we obtain:

$$\int_E (\mathbf{N}^u \bar{\Pi} \bar{\mathbf{v}}_h)^T \mathbf{N}^u \bar{\boldsymbol{\varepsilon}} dE = \int_{\partial E} (\mathbf{N}^V \bar{\mathbf{v}}_h)^T (\mathbf{N}_E \mathbf{N}^u \bar{\boldsymbol{\varepsilon}}) d\partial E \quad \forall \bar{\boldsymbol{\varepsilon}} \in \mathbb{R}^3, \quad (21)$$

where $\mathbf{N}_E$ contains the components of the outward normal $\mathbf{n} = \{n_1, n_2\}^T$, i.e.

$$\mathbf{N}_E = \begin{bmatrix} n_1 & 0 & n_2 \\ 0 & n_2 & n_1 \end{bmatrix}. \quad (22)$$

After some algebra:

$$\bar{\boldsymbol{\varepsilon}}^T \left\{ \int_E (\mathbf{N}^u)^T \mathbf{N}^u dE \right\} \bar{\Pi} \bar{\mathbf{v}}_h = \bar{\boldsymbol{\varepsilon}}^T \left\{ \int_{\partial E} (\mathbf{N}_E \mathbf{N}^u)^T \mathbf{N}^V d\partial E \right\} \bar{\mathbf{v}}_h \quad \forall \bar{\boldsymbol{\varepsilon}} \in \mathbb{R}^3, \quad (23)$$

Finally the local projector operator $\bar{\Pi}$ is:

$$\bar{\Pi} = \mathbf{G}^{-1} \mathbf{B}, \quad (24)$$

where:

$$\mathbf{G} = \int_E (\mathbf{N}^u)^T \mathbf{N}^u dE, \quad \mathbf{B} = \int_{\partial E} (\mathbf{N}_E \mathbf{N}^u)^T \mathbf{N}^V d\partial E, \quad (25)$$

We can observe that the matrix $\mathbf{G} \in \mathbb{R}^{3 \times 3}$ is computed by knowing the area of the elements $|E|$:

$$\mathbf{G} = \begin{bmatrix} |E| & 0 & 0 \\ 0 & |E| & 0 \\ 0 & 0 & |E| \end{bmatrix}, \quad (26)$$

where $|E|$ is computed using the Gauss-Green formula:

$$|E| = \int \int_E dx dy = \int_{\partial E^+} x dy, \quad (27)$$

where ∂E^+ is the boundary of the element oriented anticlockwise and the matrix $\mathbf{B} \in \mathbb{R}^{3 \times m}$:

$$\mathbf{B} = \begin{bmatrix} \int_{\partial E} n_1 \phi_1 d\partial E & 0 & \cdots & \int_{\partial E} n_1 \phi_{n_e} d\partial E & 0 \\ 0 & \int_{\partial E} n_2 \phi_1 d\partial E & \cdots & 0 & \int_{\partial E} n_2 \phi_{n_e} d\partial E \\ \int_{\partial E} n_2 \phi_1 d\partial E & \int_{\partial E} n_1 \phi_1 d\partial E & \cdots & \int_{\partial E} n_2 \phi_{n_e} d\partial E & \int_{\partial E} n_1 \phi_{n_e} d\partial E \end{bmatrix}, \quad (28)$$

where the boundary integrals in the matrix $\mathbf{B}$ are computed using the degrees of freedom of the element. In particular, the boundary integrals are computed resorting to the Gauss-Lobatto quadrature rule with $k + 1$ points, since this choice has turned to be adequate. In the case of VEM $k = 1$ we can obtain:

$$\begin{aligned} \int_{\partial E} n_1 \phi_i d\partial E &= \frac{1}{2} (n_1^{i-1} l_{i-1} + n_1^i l_i), \quad \text{for } i = 1, \dots, n_e \\ \int_{\partial E} n_2 \phi_i d\partial E &= \frac{1}{2} (n_2^{i-1} l_{i-1} + n_2^i l_i), \end{aligned} \quad (29)$$

where $l_i = |e_i|$ is the length of the i -th edge of the element E and n_j^i ($i = 1, \dots, n_e; j = 1, 2$) is the i -th outward normal of components j . Moreover if $i - 1 = 0$ use $i = n_e$ instead to $i = 0$.

The main difference between Finite Element Method and Virtual Element Method regards the approximation of the bilinear form of Eq. (14), that for the VEM is as follow

$$a_h^E(\mathbf{u}_h, \mathbf{v}_h) = \underbrace{\int_E [\Pi(\mathbf{v}_h)]^T \mathbb{C} \Pi(\mathbf{u}_h) dE}_{\bar{\mathbf{v}}_h^T \mathbf{M} \bar{\mathbf{u}}_h := \text{consistency term}} + \underbrace{S^E(\mathbf{u}_h, \mathbf{v}_h)}_{\bar{\mathbf{v}}_h^T \mathbf{K}_s \bar{\mathbf{u}}_h := \text{stability term}}, \quad (30)$$

where the first term of the right hand side is the consistent term and the second term is the stabilization term. The stabilization part is not presented in Finite Element Method and it is one of the peculiarity of the VEM. For computing the consistent term $\mathbf{M}$ we use Eq. (19) and Eq. (7)

$$\int_E [\Pi(\mathbf{v}_h)]^T \mathbb{C} \Pi(\mathbf{u}_h) dE = \bar{\mathbf{v}}_h^T \bar{\Pi}^T \left[\int_E (\mathbf{N}^u)^T \mathbb{C} \mathbf{N}^u dE \right] \bar{\Pi} \bar{\mathbf{u}}_h, \quad (31)$$

where the stiffness matrix $\mathbf{M}$ is defined as

$$\mathbf{M} = \bar{\Pi}^T \left[\int_E (\mathbf{N}^u)^T \mathbb{C} \mathbf{N}^u dE \right] \bar{\Pi}. \quad (32)$$

Eq. (32) has been rearranged in compact form as follow adopting a constant elastic tensor

$$\mathbf{M} = \bar{\Pi}^T \mathbb{C} \mathbf{G} \bar{\Pi}. \quad (33)$$

Concerning the stabilization term, we adopt the choice introduced in [38, 39]. However other authors have proposed a different stabilization terms [66]. Some preliminaries are required before introducing the stabilization term. In particular we introduce the space of the scaled monomials $\mathbf{p} \in (\mathcal{P}_k(E))^2$ since $(\mathcal{P}_k(E) \subset \mathbf{V}_h(E))^2$. In the case of VEM of degree $k = 1$ the space of the scaled monomials is

$$(\mathcal{P}_k(E))^2 = \text{span} \left\{ \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \begin{pmatrix} \xi \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \xi \end{pmatrix}, \begin{pmatrix} \eta \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \eta \end{pmatrix} \right\}, \quad (34)$$

where $\xi = (x - x_E)/h_E$, $\eta = (y - y_E)/h_E$, (x_E, y_E) are the coordinates of the centre of E and h_E its diameter. The stabilization term is defined as follow

$$\mathbf{K}_s = \tau \text{tr}(\mathbf{M}) \left[\mathbf{I} - \mathbf{D} (\mathbf{D}^T \mathbf{D})^{-1} \mathbf{D}^T \right], \quad (35)$$

where $\tau \in \mathbb{R}$ is a coefficient defined by the user that can be set equal to $1/2$ for linear elasticity [65] and $\text{tr}(\cdot)$ denotes the trace operator. The matrix $\mathbf{D} \in \mathbb{R}^{m \times 6}$ collects the values of the polynomials $\mathbf{p}_i$ at the degrees of freedom on E (nodes
280 of the element in the case of degree $k = 1$). An accurate inspection of Eq. (35) reveals that the stability term is basically a rough approximation of the internal energy associated with the difference between VEM shape function and its projection, while $\tau \text{tr}(\mathbf{M})$ scales the term with respect to the consistency part, which is the properly used for providing convergence of the method [38].

285 3.0.4. Local load vector

Regarding the approximation of right hand side of the equation (13), the same assumption proposed in [65] is used, i.e.

$$\mathcal{F}(\mathbf{v}_h) = \left(\int_E \mathbf{f} dE \right)^T \sum_{i=1}^{n_e} \frac{1}{n_e} \mathbf{v}_h(v_i), \quad (36)$$

so that the body load over the element E is subdivided over all nodes v_i of the polygonal element.

4. Numerical Results

In this section, the results of parametric analyses performed using the described
 290 computational FSHP in conjunction with VEM are provided. We restrict our
 investigation to polycrystalline material with thin interfaces, since the other
 type of composite has been already extensively studied in [67, 58, 68].

First, the reliability of the assumptions for the mesh topology, i.e. using one vir-
 tual element to model the grain and several triangular virtual elements to model
 295 the thin interfaces, is investigated by comparing the results with those obtained
 via a very dense triangular finite element mesh. Two distinct cases are studied:
 material A with stiff grains in softer interfaces and, material B with soft grains
 in stiffer interfaces. The analyses are performed for different level of material
 contrasts, c , between the Young moduli of constituents (inclusions/matrix). In
 300 the case of polycrystal materials the grains and interface layers play the role of
 inclusions and matrix, respectively.

4.1. Comparison between VEM and FEM discretization

As a preliminary test, we consider an ideal material that mimics a cermet-like
 composite with grains and thin interfaces and investigate, for a given window
 305 size, the results obtained via VEM and FEM discretizations. We consider the
 window size $L = 100 \mu m$, the average dimension of grains and the thickness
 interfaces equal to $\bar{d} = 40 \mu m$ and $s = 2 \mu m$, respectively. The elastic moduli
 of the interface layer are $E_m = 1.0 MPa$ and $\nu_m = 0.25$, while for the grains
 $E_i = 1, 2, \dots, 10 MPa$ and $\nu_m = 0.25$.

The components of the homogenized elastic tensor $\bar{\mathbb{C}}_{ijhk}$ are evaluated using
 both Dirichlet (apex D) and Neumann (apex N) boundary conditions. The
 structure of the computed homogenized stiffness matrix is equal to:

$$\bar{\mathbb{C}} = \begin{bmatrix} \bar{\mathbb{C}}_{1111} & \bar{\mathbb{C}}_{1122} & 0 \\ \bar{\mathbb{C}}_{2211} & \bar{\mathbb{C}}_{2222} & 0 \\ 0 & 0 & \bar{\mathbb{C}}_{1212} \end{bmatrix}. \quad (37)$$

310 More specifically, the results obtained using with virtual elements are compared to those obtained using finite elements, see Fig 7(b) for details on the mesh used. The FEM mesh adopted for the simulation has 15749 #Nodes, while the VEM mesh has 3493 #Nodes.

Figure 7: Example of the meshes adopted: FEM mesh (a) and VEM mesh (b)

In Tabs. 1 and 2 the homogenized moduli obtained for different level of contrast have been reported ($1 \leq E_i/E_m \leq 10$) using both Dirichlet and Neumann boundary conditions, respectively. The solution obtained adopting the VEM mesh is always close to the reference solution FEM. The maximum errors, computed as $e = (\overline{\mathbb{C}}_{ijhk}^{FEM} - \overline{\mathbb{C}}_{ijhk}^{VEM}) / \overline{\mathbb{C}}_{ijhk}^{FEM}$, in the case of the highest contrast considered, $E_i/E_m = 10$, are 0,79% and 0.17% for $\overline{\mathbb{C}}_{2222}^D$ and $\overline{\mathbb{C}}_{1111}^N$, respectively.

320 The obtained results highlight the high performance of the VEM methodology in these applications. VEM preserves $\sim 300\%$ of the degrees of freedom respect to the FEM with consequent reduction of the computational burden.

4.2. FSHP applied to materials A and B

In this example we take into account both materials A (stiff grains) and B (soft grains) with elastic properties reported in Tab. 3, where also the contrast c is reported, and the average dimension of grains and the hard-core have been fixed equal to $\bar{d} = 40 \mu m$ and $s = 2 \mu m$, respectively.

As an example, in Fig. 8 the variation of the average bulk modulus $\langle \mathbb{K} \rangle$ with respect to the number of simulations has been shown for different values of window size L . As expected, when the dimension of the window size increases, the

330

<i>Homogenized moduli</i>						
c E_i/E_m	Type	$\overline{\mathbb{C}}_{1111}^D$	$\overline{\mathbb{C}}_{1122}^D$	$\overline{\mathbb{C}}_{2211}^D$	$\overline{\mathbb{C}}_{2222}^D$	$\overline{\mathbb{C}}_{1212}^D$
1	VEM	1.2000	0.4000	0.4000	1.2000	0.8000
	FEM	1.2000	0.4000	0.4000	1.2000	0.8000
2	VEM	2.0890	0.6869	0.6868	2.0929	1.3744
	FEM	2.0909	0.6868	0.6869	2.0948	1.3767
3	VEM	2.8116	0.9059	0.9060	2.8251	1.8140
	FEM	2.8179	0.9059	0.9062	2.8313	1.8210
4	VEM	3.4149	1.0791	1.0799	3.4411	2.1618
	FEM	3.4265	1.0792	1.0804	3.4529	2.1739
5	VEM	3.9287	1.2202	1.2223	3.9695	2.4438
	FEM	3.9460	1.2204	1.2229	3.9873	2.4607
6	VEM	4.3734	1.3377	1.3416	4.4296	2.6769
	FEM	4.3965	1.3379	1.3423	4.4535	2.6981
7	VEM	4.7634	1.4376	1.4437	4.8355	2.8728
	FEM	4.7921	1.4377	1.4442	4.8653	2.8975
8	VEM	5.1094	1.5237	1.5324	5.1973	3.0395
	FEM	5.1435	1.5236	1.5327	5.2329	3.0671
9	VEM	5.4193	1.5991	1.6106	5.5228	3.1830
	FEM	5.4586	1.5986	1.6104	5.5638	3.2129
10	VEM	5.6992	1.6657	1.6802	5.8180	3.3077
	FEM	5.7434	1.6648	1.6794	5.8642	3.3395

Table 1: Homogenized moduli obtained by applying Dirichlet boundary conditions

<i>Homogenized moduli</i>						
c E_i/E_m	Type	$\overline{\mathbb{C}}_{1111}^N$	$\overline{\mathbb{C}}_{1122}^N$	$\overline{\mathbb{C}}_{2211}^N$	$\overline{\mathbb{C}}_{2222}^N$	$\overline{\mathbb{C}}_{1212}^N$
1	VEM	1.2001	0.4003	0.4003	1.2001	0.8000
	FEM	1.2001	0.4004	0.4004	1.2001	0.8000
2	VEM	2.0971	0.6930	0.6930	2.1005	1.4637
	FEM	2.0970	0.6927	0.6927	2.1006	1.4637
3	VEM	2.8364	0.9215	0.9215	2.8488	2.1273
	FEM	2.8361	0.9208	0.9208	2.8488	2.1273
4	VEM	3.4588	1.1031	1.1031	3.4836	2.7910
	FEM	3.4579	1.1021	1.1021	3.4832	2.7910
5	VEM	3.9912	1.2496	1.2496	4.0303	3.4546
	FEM	3.9894	1.2484	1.2484	4.0292	3.4546
6	VEM	4.4525	1.3695	1.3695	4.5071	4.1183
	FEM	4.4494	1.3684	1.3684	4.5047	4.1183
7	VEM	4.8563	1.4688	1.4688	4.9269	4.7819
	FEM	4.8517	1.4680	1.4680	4.9230	4.7819
8	VEM	5.2131	1.5520	1.5520	5.2998	5.4456
	FEM	5.2067	1.5516	1.5516	5.2941	5.4456
9	VEM	5.5308	1.6223	1.6223	5.6335	6.1092
	FEM	5.5226	1.6224	1.6224	5.6258	6.1092
10	VEM	5.8155	1.6823	1.6823	5.9339	6.7729
	FEM	5.8055	1.6830	1.6830	5.9241	6.7729

Table 2: Homogenized moduli obtained by applying Neumann boundary conditions

<i>Material</i>	$c = E_i/E_m$	E_m [MPa]	E_i [MPa]	ν_m	ν_i
A10	10	1000	10000	0.25	0.23
A100	100	100	10000	0.25	0.23
B01	0.1	10000	1000	0.25	0.23
B001	0.01	10000	100	0.25	0.23

Table 3: Mechanical properties adopted

number of simulations, required to archive the convergence, decreases. Accordingly to the convergence criterion adopted (see Section 2.2), the convergence is obtained for a given small value of the number of simulations, N^{lim} .

In Figs. 9(a) and 9(b), the average values of the homogenized bulk modulus, $\langle \mathbb{K} \rangle$, obtained for increasing window size, L , are reported.

The convergence trend for the different materials depends on the different dispersion of results, as shown in Fig. 10 and Fig. 11, where the Coefficient of Variation, $CV(\mathbb{K})$, is also plotted for several values of window size L for Dirichlet (blue solid line) and Neumann (red solid line) BVPs.

5. Final Remarks

In this paper we present an efficient extension of the Fast Statistical Homogenization (FSHP), previously developed by the authors for the homogenization of particle composites in [36, 37, 69], to account for the peculiar geometry of the polycrystal and composites with grains and thin interfaces. The Virtual Element Method is used as numerical tool to solve the partial differential equations governing the elastic problem. Starting from a random polygonal mesh, a novel automatic procedure to insert thin interfaces between grains is presented. Each grain is discretized using a single VEM, while the interfaces zones present a dense triangular mesh (exploiting Delaunay triangulation). Clear advantages in terms of computational burden are found with respect to the Finite Element Method (saving of about 350% of degrees of freedom). This circumstances are particularly favourable in cases of materials with very high or very low contrasts,

(a) Dirichlet boundary conditions

(b) Neumann boundary conditions

Figure 8: Material type B01: average bulk modulus $\langle \mathbb{K} \rangle$ versus the number of simulations n for different window sizes L .

for which large window domains are required, as reported in [30, 19, 34, 9].

The results shown for a set of ideal materials, characterized by different mis-
355 matches between elastic moduli of grains and interfaces (material contrast),
confirm the reliability and the efficiency of the statistical procedure in conjunc-

(a) Material type A

(b) Material type B

Figure 9: Average bulk modulus $\langle \mathbb{K} \rangle$ versus different window sizes L : material type A (a) and material type B (b).

(a) Material type A10

(b) Material type A100

Figure 10: Coefficient of variation $CV(\mathbb{K})$ for different window sizes L : material type A.

tion with the innovative method of Virtual Elements Method.

Here, the analyses are limited to the Cauchy continuum and the extension to enriched non-classical continua, such as Couple-Stress and Cosserat, [34], in

(a) Material type B01

(b) Material type B001

Figure 11: Coefficient of variation $CV(K)$ for different window sizes L : material type B.

360 order to better describe the behaviour of micro-structured material, is one of the future developments. Moreover, we will upgrade the procedure to take into account possible anisotropic behaviours, since this type of materials are gener-

ally characterized by anisotropic properties, that varies grain-by-grain. Another interesting application and future development will be applying the procedure
365 for the design of new materials with prescribed mechanical characteristics.

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