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Virtual Element Method: micro-mechanics applications

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Abstract. In this contribution we present an application of the lowest order Virtual Element Method (VEM) to the problem of material computational homogenization. Material homogenization allows retrieving material properties through suitable volume averaging procedures, starting from a detailed representation of the micro-constituents of the considered material. The representation of such microstructure constitutes a remarkable effort in terms of data/mesh preparation, especially when there is not evident microstructural regularity. For such a reason, computational micromechanics may represent a challenging benchmark for showing the potential of VEM. In this contribution, polycrystalline materials are considered as an application. The proposed technique constitutes a first step towards modelling of damage processes in micro-structured materials.

Introduction

The Virtual Element Method (VEM) [1] is currently emerging as a powerful and robust generalization of the Finite Element Method (FEM). One of the important features of the VEM is its ability to deal with very general polygonal/polyhedral meshes, which ensures a noticeable simplification in the data preparation stage of the analysis that often is much user dependent and may have a deep influence on the quality and objectivity of the analysis results.

In this contribution, we present an application of the lowest order VEM to the problem of material computational homogenization, which is a process that allows to retrieve material properties through suitable volume averaging procedure starting from a detailed representation of the micro-constituents of the considered materials, such as fibers and matrix in composite materials or crystals in polycrystalline metallic or ceramic materials. The representation of the materials microstructure constitutes a remarkable effort in terms of data and mesh preparation, especially when there is not evident microstructural regularity. For such a reason, computational micromechanics may represent a challenging benchmark for showing the potential of VEM.

In this work, polycrystalline materials are considered as an application. Polycrystalline materials, either metals or ceramics, are extensively employed in several engineering applications, including the manufacture of micro-electro-mechanical systems and devices (MEMs), which further justifies the interest towards computational micromechanics. Polycrystalline silicon, or polysilicon, for example, is used in MEMS components. The polycrystalline microstructure is characterized by the morphology and crystallography of the grains and by the physical and chemical properties of the inter-granular interfaces, which play an important role in their micro-mechanics.

Several computational techniques have been developed for the analysis of polycrystalline micromechanics, including their damage and failure behavior. Grain-scale models have been developed for material homogenization, quasi-static failure, stress corrosion cracking and fatigue, employing either the finite element method (FEM) [2-4], integral formulations [5-14] or other techniques [15,16]. In all the mentioned works, the preparation of suitable morphological representations of the microstructure and its meshing cause non-trivial concerns [17]. In fact, such micro-morphologies exhibit several statistical features that may pose remarkable issues for the generation of quality meshes for subsequent numerical analysis.

First order approximations of general polycrystalline aggregates are often generated resorting to Voronoi tessellations [17], which are built starting from seeds randomly scattered within a selected bounding region. It has often been highlighted how the random nature of such morphologies

requires extraordinary robustness of the pre-processing meshing algorithms. In this respect, the inherent flexibility offered by the VEM may constitute a valuable asset. Clipped Voronoi tessellations are used to generate polycrystalline representative volume elements also in the present work and the effective linear elastic properties of aggregates of grains with cubic crystallographic symmetry are then determined through computational homogenization on such unit cells. By comparing the results of the numerical simulations with first-order bounds and experimental data we show the reliability of the proposed homogenization technique.

In the following sections, the basic concepts of the VEM are first recalled. Some details about the multi-region implementations and the advantages provided by the specific features of the method are then discussed, before the numerical application to computational homogenization in the last section.

Low order VEM for 2D elastic microstructures

The basic concepts of the Virtual Element method are briefly recalled here for the sake of completeness. However, the focus in the present work is on the features of the method that can be profitably exploited in the analysis of complex heterogeneous microstructures. For more theoretical mathematical foundations the reader is referred to [1, 18-21].

The Virtual Element Method is a generalization of the Finite Element Method to general polygonal or polyhedral meshes. The main feature of the VEM is that, on each element, the trial and test functions contain all the polynomial up to a given degree *k* plus other additional functions that, in general, are not polynomials and are solutions, within the element, of a boundary value problem. These additional functions are explicitly known only on the element edges while, inside each element, they are not explicitly known and never computed. Thus they are said to be *virtual*. The local discrete bilinear form and linear functionals of the variational formulation are computed by substituting the virtual test and trial functions and their gradients with their polynomial projections. Through a particular choice of the degrees of freedom, these projections are exactly computed *directly from the degrees of freedom* without actually solving the local boundary value problem.

Virtual element method fundamentals. Let us consider a 2D linear elastic problem set in the framework of small strains. The elastic body lays within the domain $\Omega \subset \mathbb{R}^2$ with boundary $\Gamma = \partial\Omega$. In general, the body is subjected to the volume forces $\mathbf{f}(\mathbf{x})$ where the argument denotes the position coordinates in vector format. In the following, homogeneous Dirichlet boundary conditions are assumed for the sake of conciseness. However, other kinds of boundary conditions can be easily treated using standard FEM procedures. Classically the finite element formulation for elasticity can be built starting from the principle of virtual work, which provides the weak form from which the discrete operators are obtained after suitable discretization. In particular, the solution **u** is sought so that

$$\int_{\Omega} \mathbf{C}\cdot\boldsymbol{\varepsilon}(\mathbf{u})\cdot\boldsymbol{\varepsilon}(\delta\mathbf{v})\,d\Omega = \int_{\Omega} \mathbf{f}\cdot\delta\mathbf{v}\,d\Omega \qquad \forall\delta\mathbf{v}\in\mathbf{V}\subset\left[H_0^1(\Omega)\right]^2 \tag{1}$$

where $\mathbf{V}$ is the space of the kinematically admissible infinitesimal displacements and H_0^1 is the first order Sobolev space, comprising functions square integrable on Ω up to the first order derivative. In the above weak form, linear elastic constitutive behavior has been assumed, together with the small deformation strain-displacements relationships. To solve the elastic problem, the analysis domain is sub-divided into a collection of non-overlapping polygons *E*. One of the features of the VEM is that, unlike the FEM, it allows the choice of very general polygons, including non-convex ones. Once a generic partitions into finite elements has been selected, it is possible to define, for each element, the following space of local admissible displacements as

$$\mathbf{V}_{h,E} = \left\{ \mathbf{v}_h \in \left[H^1(E)\cap C^0(E)\right]^2 : \mathbf{v}_{h,\partial E}\in\left[C^0(\partial E)\right]^2, \mathbf{v}_{h,e}\in\left[P_1(E)\right]^2 \ \forall e\in\partial E, \Delta\mathbf{v}_h = \mathbf{0} \text{ in } E \right\} \tag{2}$$

where $P_1(E)$ is the space of linear polynomials on E and Δ denotes the component-wise Laplacian operator. We observe that, unlike the classical FEM, the space $\mathbf{V}_{h,E}$ is not entirely explicitly defined. In fact, it is made of vector-valued harmonic functions $\mathbf{v}_h$ that are explicitly known only on the element edges, where they are globally continuous and, in the case of the first order VEM, linear polynomials. Inside the element, $\mathbf{V}_{h,E}$ contains all linear polynomials of first order plus other functions that are not explicitly known. Consequently, it is not possible to explicitly define local shape functions as in the standard FEM. In contrast, VEM uses approximated shape functions whose point-wise value is determined by a suitable choice of the degrees of freedom. For the first-order VEM here considered, the degrees of freedom are the point-wise values of $\mathbf{v}_h$ at each vertex of the generic polygonal element *E*. The global discrete space of admissible displacements $\mathbf{V}_h$ is obtained by assembling all the local spaces $\mathbf{V}_{h,E}$.

The restriction of the continuous variational formulation to the space $\mathbf{V}_h$ implies finding $\mathbf{u}_h \in \mathbf{V}_h$ such that Eq.1 is satisfied $\forall \mathbf{v}_h \in \mathbf{V}_h$. Since the functions $\mathbf{v}_h$ are not explicitly known within the generic element *E*, the integral

$$\int_E \mathbf{C}\cdot\boldsymbol{\varepsilon}(\mathbf{u}_h)\cdot\boldsymbol{\varepsilon}(\delta\mathbf{v}_h)\,dE \tag{3}$$

cannot be computed by numerical integration, as it is usually done. The Virtual Element Method proceeds by introducing the projection operator $\Pi_E : \mathbf{V}_{h,E} \to \left[P_1(E)\right]^2$ that is used to compute the linear polynomial projection of any function $\mathbf{v}_h \in \mathbf{V}_{h,E}$ [18]. The projection operator Π_E is defined on each element by the following orthogonality condition:

$$\int_E \mathbf{C}\cdot\boldsymbol{\varepsilon}(\mathbf{p})\cdot\boldsymbol{\varepsilon}(\delta\mathbf{v}_h - \Pi_E\delta\mathbf{v}_h)\,dE = 0 \quad \forall \mathbf{p} \in \left[P_1(E)\right]^2. \tag{4}$$

The projector Π_E can be exactly evaluated, as the integrals involved in Eq.4 can be computed by just knowing the values of $\mathbf{v}_h$ on the element edges, after using the integration by parts. For the lowest order VEM, it can be shown how such integrals can be computed by using just the knowledge of the values of $\mathbf{v}_h$ at the element vertices, see [19].

Once the projection operator is defined and computed, Eq.3 can be expressed as:

$$\int_E \mathbf{C}\cdot\boldsymbol{\varepsilon}(\mathbf{u}_h)\cdot\boldsymbol{\varepsilon}(\delta\mathbf{v}_h)\,dE = \int_E \mathbf{C}\cdot\boldsymbol{\varepsilon}(\Pi_E\mathbf{u}_h)\cdot\boldsymbol{\varepsilon}(\Pi_E\delta\mathbf{v}_h)\,dE + S^E(\mathbf{u}_h, \delta\mathbf{v}_h) \tag{5}$$

The first term on the right-hand side of Eq.5 is the part of the local stiffness matrix that ensure the *consistency* property [1]. The second term $S^E(\mathbf{u}_h, \delta\mathbf{v}_h)$ is a *stabilization* term used to preserve the positive definitiveness of the energy local bilinear form (the local virtual work) [1,20] and it can be computed as suggested in [21]. Once the contribution of each element to the global stiffness matrix is computed using Eq. they are assembled into the global stiffness matrix as in the standard FEM. The right-hand side loading term, for the lowest order VEM here considered, can be approximated by applying an integration rule based on vertexes [21].

Multi-region implementation for micromechanics. The key features of the VEM useful in the treatment of complex analysis domains are:

- The elemental contributions to the global stiffness matrix, *in the case of the lowest order formulation*, can be computed by resorting to the values of the unknown displacement field at the corners of the polygonal elements;

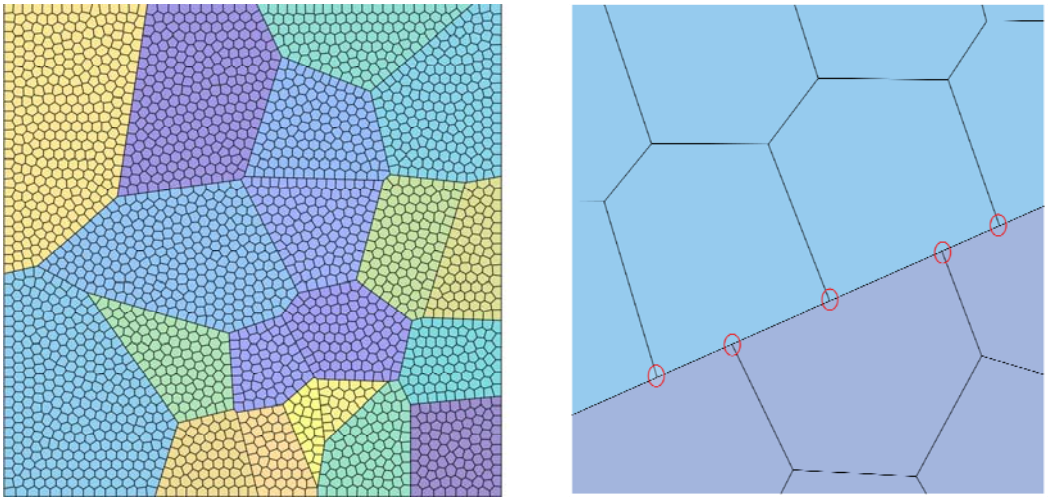
- Since the explicit knowledge of the shape functions within the element is not required, general polygonal elements can be easily treated, without resorting to complex numerical integration algorithms;
- In particular, the VEM allows treating also non-convex polygonal elements and polygonal elements *with aligned consecutive edges*; the latter feature allows to easily by-pass the meshing complexities induced by the presence of *hanging nodes*.

The above features are particularly suitable for the treatment of multi-region problems, which typically occur in micro-mechanics analyses, as it will be better described in the next application to the analysis of polycrystalline materials.

Polycrystalline computational homogenization

Using the implementation of the described low-order VEM formulation, numerical simulations have been performed to estimate the effective elastic properties, namely the isotropic Young's modulus E and shear modulus G, of polycrystalline specimens. In this work, such estimation is performed in accordance with the homogenization procedure described in [7]: *a*) polycrystalline morphologies are generated by Voronoi tessellations; *b*) each grain within the polycrystalline microstructure is independently meshed and modeled using the VEM; *c*) after meshing and matrix assembly for the individual grains, suitable inter-granular continuity conditions are enforced; *d*) each polycrystalline specimen is then subjected to three linearly independent sets of boundary conditions (two elongations and one shear); *e*) the strain and stress fields are averaged over the aggregate overall volume and the link between averaged stress and strains provides an estimation of the effective elastic constants. Once a certain number of grains N_g is selected, the above procedure is applied to a certain number of microstructures, so to average the fields of interest over different realizations, in a framework of statistical homogenization.

Copper, whose single crystals exhibit cubic crystallographic symmetry, is considered as benchmark material. Copper's three independent elastic constants are $C_{11} = 168.4$ GPa, $C_{12} = 121.4$ GPa and $C_{44} = 0.75$ GPa. A sample polycrystalline microstructure, generated by Voronoi tessellation, after initially selecting the number of grains N_g, is shown in Fig.1a. Morphologies with N_g = 10, 20, 50, 100, 200 grains have been considered and, for each selected number of grains, 50 different morphologies have been considered.



(*a*) (*b*)

Fig.1: a) Example micro-morphology generated by Voronoi tessellation and its associated mesh; b) Interface hanging nodes as additional VEM nodes of polygonal elements with parallel contiguous edges.

Fig.1a shows an example mesh of a 20-grain morphology, while Fig.1b illustrates one of the advantages provided by the VEM in the meshing of the polycrystalline microstructure. The interface between two different generic grains is shown: the two grains are independently meshed and this circumstance would require, in the case basic FEM was used, a careful choice of conformal mesh elements, so to restore displacements continuity and tractions equilibrium through conditions imposed at the interface matching nodes. On the other hand, being able to deal with polygonal elements of any order, even with parallel contiguous edges, the VEM by-passes the requirement of conformal meshing by treating the arising mismatched *hanging* nodes as additional nodes within the common edge for each of the interested interface elements, then providing a simple and elegant solution to the interface meshing complexity. Each grain can then be independently meshed, without mesh constraints induced by the surrounding grains; possible hanging nodes are easily treated as additional edge nodes between contiguous parallel edges of interfaces polygonal elements.

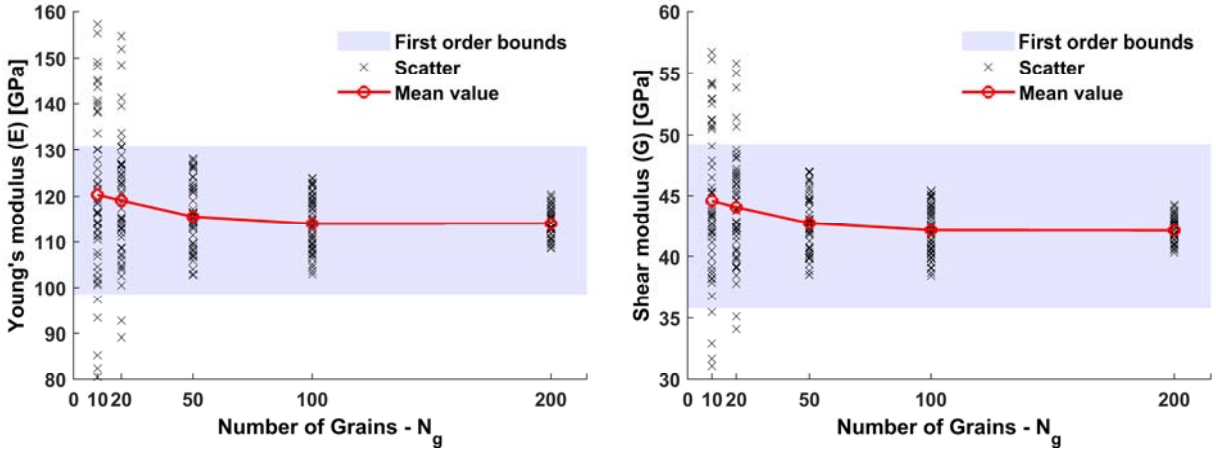


Fig.2: Effective elastic constants of copper as computed by the VEM-based homogenization scheme.

The results of the proposed homogenization scheme are reported in Fig.2, where also the first order bounds are shown. It is noted how the scatter of the effective properties decreases as the number of grains within the considered realizations increase.

Summary

In this work, the advantages provided by the low-order Virtual Element Method in the analysis of a micro-mechanical homogenization problem are described and discussed. It is shown as the features of VEM allow to by-pass complexities arising in the mesh of random polycrystalline micro-structures, considered as example material. The computed effective properties of polycrystalline copper have eventually confirmed the effectiveness of the VEM-based computational homogenization approach.

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