The Virtual Element Method for the numerical homogenization of electro-mechanical responses

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The virtual element method (VEM) has been attracting interest for applications in micromechanical homogenization. This work aims to introduce and analyze multiphysical formulations in a VEM-based numerical homogenization scheme. Addressing electromechanical polycrystalline materials, the performance of a VEM-based approach with respect to FEM-based approaches is investigated. Results show the outperformance of VEM with respect to FEM models (with the same number of degrees of freedom) on the obtained value of homogenized quantities. The coarse mesh permitted by the VEM rationale, where each grain might represent one element, allows to maintain a low computational cost with a high accuracy.

1 Introduction

The computational homogenization of the mechanics of polycrystalline materials is associated with requests of flexibility with regards to mesh generation and element shapes. This request couples with the challenge of treating strong and random anisotropies associated with different crystalline systems. In addition, advanced engineering applications (like the design of sensors, batteries or storage moduli) introduce the need of accounting for electromechanical coupling effects. In the framework of micromechanical homogenization, the virtual element method (VEM) has been attracting attention for modeling anisotropic material behaviors and for the homogenization of composite materials [1–4]. This method permits the use of polygonal/polyhedral elements which might perfectly fit grain geometries in polycrystalline materials. Present works aims to analyze the performance of VEM-based homogenization for multiphysical polycristalline materials, extending results shown in [4] in an electromechanical context and by comparing FEM and VEM approaches also in a three-dimensional framework.

2 Constitutive Framework and Computational Approach

At the microscale, a representative volume element $\mathcal{RVE}$ of an electro-mechanical polycrystalline material is introduced. From the primary variables of the coupled problem (i.e. displacement $\mathbf{u}$ and electric potential ϕ), the strain $\boldsymbol{\varepsilon}$ and electric $\mathbf{E}$ fields immediately follows and are collected in vector $\mathbf{P} = \text{vec}\{\boldsymbol{\varepsilon}, \mathbf{E}\}$. Each grain is anisotropic and the grain material preferred directions are identified by a pseudo-random set of angles $\Phi_i \in [0, 2\pi]$ for $i \in \{1, 2, 3\}$. For each grain, running over index g, the constitutive response is introduced through a quadratic potential energy density $\psi_g(\mathbf{P})$:

$$\psi_g(\mathbf{P}) = \frac{1}{2}\mathbf{P} \cdot \mathbb{G}_g \cdot \mathbf{P}, \qquad \mathbb{G}_g = \mathbb{III}_{\mathbf{L}}^{-1}\mathbb{G}_l\mathbb{III}_{\mathbf{P}}, \qquad \{\mathbb{III}_{\mathbf{L}}, \mathbb{III}_{\mathbf{P}}\} \in \mathcal{SO}(3)\,. \tag{1}$$

Here, $\mathbb{G}_l$ denotes the overall modulus of the physical coupled problem, collecting moduli $\{\mathbb{C}, \mathbf{e}, \boldsymbol{\epsilon}\}$ representing the mechanical, electro-mechanical, and dielectric moduli, respectively. These moduli are expressed in a coordinate system aligned with grain material preferred directions. Thus, $\mathbb{G}_l$ is rotated back into a global coordinate system at the $\mathcal{RVE}$ level by means of suitable coordinate-transformation tensors $\{\mathbb{III}_{\mathbf{L}}, \mathbb{III}_{\mathbf{P}}\}$. The homogenized moduli are obtained by a series of numerical simulations. By exploiting the average strain theorem, generalized in a multiphysics framework [5], appropriate boundary conditions at $\mathcal{RVE}$ level are applied in order to obtain an orthonormal basis for the average primary variables within the $\mathcal{RVE}$. Therefore, introducing $\langle\cdot\rangle$ as the volume average operation within the $\mathcal{RVE}$, 9 independent values $\langle\mathbf{P}\rangle = \bar{\mathbf{P}}_m$ are imposed, such that $[\bar{\mathbf{P}}_m]_i = \delta_{im}$, with δ_{im} being the delta-Kronecker symbol ($i, m = 1, \ldots, 9$). The homogenized moduli are obtained by volume averaging of the output quantities obtained for all $\bar{\mathbf{P}}_m$, that is stress $\boldsymbol{\sigma}|_{\bar{\mathbf{P}}_m}$ and electric displacement $\mathbf{D}|_{\bar{\mathbf{P}}_m}$

$$[\overline{\mathbb{G}}]_{im} = [\text{vec}\{\boldsymbol{\sigma}_{av}, \mathbf{D}_{av}\}]_{im} \quad \text{with} \quad \boldsymbol{\sigma}_{av} = \langle\boldsymbol{\sigma}|_{\bar{\mathbf{P}}_m}\rangle\,, \;\; \mathbf{D}_{av} = \langle\mathbf{D}|_{\bar{\mathbf{P}}_m}\rangle\,, \;\; \text{and} \;\; i, m = 1, \ldots, 9\,. \tag{2}$$

As outlined in [4], virtual elements provide with the ability of being arbitrary shaped and thus also to be able of handling varying number of nodes. This leads to a perfect fit regarding artificially generated polycrystalline grain structures through Voronoi tessellation, where each grain might be represented by a single element. The virtual element approach employs a split of primary fields $\mathfrak{U} = \{\mathbf{u}, \phi\}$ into projected part and a remainder $\mathfrak{U} = \mathfrak{U}_h + (\mathfrak{U} - \mathfrak{U}_h)$. The latter induces a split of the potential into a consistency and a stabilization part [4], with a control-parameter $\beta \in [0, 1]$ for stabilization-influence. Following results in [4], the latter parameter is chosen equal to $\beta = 0.1$.

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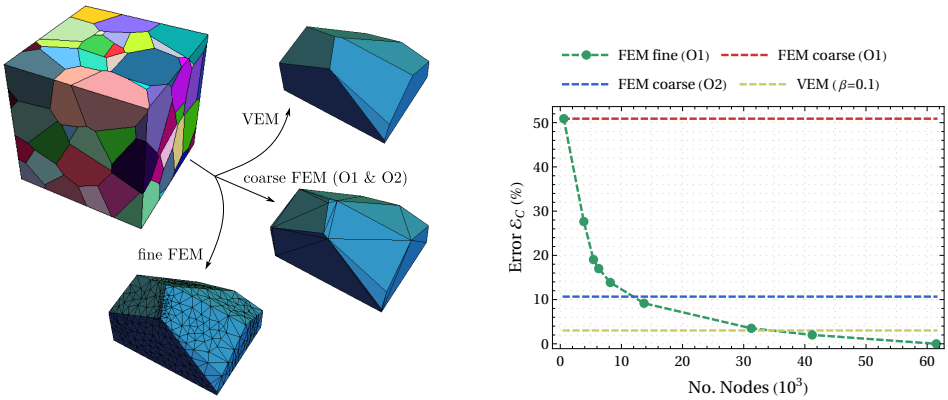
3 Results

Numerical results compare solutions obtained with different classical FEM approaches and a low-order VEM solution. In the VEM case, each element represents one grain (possibly non-convex) and nodes are located only at grain vertices. Moreover, a low-order FEM coarse O1 mesh is introduced (with linear shape function and the same number of nodes as the VEM one), together with a higher order FEM coarse O2 mesh (with quadratic shape functions and the same number of elements as FEM coarse O1). A quantitative comparison is obtained introducing the computational error $\mathcal{E}_C$:

$$\mathcal{E}_C = 10^2 \left| \frac{||\overline{\mathbb{G}}||^{\mathcal{M}}}{||\overline{\mathbb{G}}||^{fine}} - 1 \right|, \qquad || \, (\cdot) \, || = \sqrt{\sum_i^n \sum_j^m (\cdot)_{ij}^2}, \qquad \mathcal{M} = \{\text{FEM (O1), FEM (O2), VEM}\}. \tag{3}$$

The computational error $\mathcal{E}_C$investigates on the percentage of deviation of the coupled electromechanical modulus $\bar{\mathbb{G}}$ with respect to a FEM-based fine solution $(\cdot)^{fine}$ obtained from a convergence study on the FEM simulation (> 300k elements).



(a) $\mathcal{RVE}$ and meshed polyhedral element (b) Computational error

Fig. 1: (a) $\mathcal{RVE}$ and one polyhedral shaped grain, discretized by one virtual element, and by coarse or fine tetrahedral finite elements; (b) Computational error $\mathcal{E}_C$ on the Frobenius Norm of homogenized modulus $\overline{\mathbb{G}}$ of the electro-mechanical coupled problem for a piezoelectric material with trigonal unit cell structure. Values of parameters correspond to material mp-1434 in the Materials Project [6].

Results show that the Virtual Element (VE) formulation allows to accurately capture the coupled electro-mechanical behavior of the polycrystalline assembly. In particular, Fig. 1b demonstrates that the computational error on $\overline{\mathbb{G}}$ obtained with a VE-approach is significantly less than the one obtained with the linear coarse FE-approach (3% vs 50%). Even when applying a higher order finite element formulation on the coarse FE mesh, the VEM solution provides a lower error with respect to the finest benchmark solution (3% vs 10%). The results were obtained by using the symbolic-numeric software tools AceGen/AceFEM [7], a subpackage of Mathematica, which utilizes automatic differentiation based formulation techniques.

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