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An adaptive curved virtual element method for the statistical homogenization of random fibre-reinforced composites

E. Artioli [a,*], L. Beirão da Veiga [b], M. Verani [c]

[a] Department of Civil Engineering and Computer Science, University of Rome Tor Vergata, Via del Politecnico 1, Rome, Italy
[b] Department of Mathematics and Applications, University of Milano Bicocca, Milan, Italy
[c] MOX-Department of Mathematics, Politecnico di Milano, Milan, Italy

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ABSTRACT

We propose an adaptive curved virtual element method (ACVEM) which is able to combine an exact representation of the involved computational geometry and a dynamic tuning of the optimal mesh resolution through a robust and efficient residual-based a-posteriori error estimator. A theoretical analysis on the reliability of the estimator and a gallery of numerical tests supports the efficacy of the proposed approach. The ACVEM is combined with Monte Carlo simulations, and a methodology is developed to determine homogenized material moduli and representative unit cell size of random long-fibre reinforced composites in the framework of antiplane shear deformation. Accuracy and computational efficiency of the proposed homogenization procedure is confirmed by numerical examples.

1. Introduction

Composite materials are extensively used materials in many engineering applications due to their interesting properties, as, for instance, high strength-to-weight ratio and tunable features of the constituents. Use of such complex materials requires accurate yet computationally efficient methods of analysis of their mechanical response.

In reference to the scope of the present communication which focuses on *fibre reinforced* composite materials, a large number of analysis methods have been devised seeking to approximate composite structural mechanics by analyzing a representative (smaller) part of the composite microstructure, commonly called a Representative Volume Element (RVE) or Representative Unit Cell (RUC) [1,2]. They all are based on scale decoupling leading to analyses at the local and global levels and, with some differences, apply either to doubly periodic arrangements of fibres (doubly periodic composites) or random distributions of inclusions (random composites) within a matrix medium. The local level analysis models the microstructural details to determine effective elastic properties. The composite structure is then replaced by an equivalent homogeneous material having the calculated effective properties. Such a process of calculating effective properties is usually termed *material homogenization* [3] and has led to massive interest in the scientific community since the early 70s [3–11].

In this regard, a significantly studied method for solving the micro scale problem is represented by *asymptotic homogenization* which can lead, in selected cases, such as linear elastic material response and periodic arrangement of the inclusions, to closed form solutions of the homogenization problem. Despite asymptotic homogenization or other methods are used to solve the small scale problem, in a wide variety of situations homogenization requires an approximate numerical solution of the relevant homogenized field equation [12–14]; such is the case of composite materials whose constituents exhibit complex constitutive behavior [15–20]. Another typical case requiring a numerical approximation is that of composites with inclusions having random size and shape, as well as random space distribution within the host medium. In the latter case, the assessment of homogenized quantities will require in general a twofold procedure: on the one hand, a numerical approach for the solution of the field equation under investigation and computation of relevant homogenized properties, and, on the other hand, a statistical evaluation of such quantities by some sort of averaging procedure over a sufficiently large set of random realizations. An efficient statistical homogenization procedure of random composite materials hence requires high accuracy level of the numerical solution of the field equation for each realization, in order to converge rapidly, as pointed out, for instance, by Kanit and Forest in their pioneering work, where a parallelized computational procedure is presented to tackle these critical

* Corresponding author.
E-mail address: artioli@ing.uniroma2.it (A. Artioli), (L. Beirão da Veiga), shuang.zhang@colorado.edu (M. Verani).

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issues [21]. The finite element method is undoubtedly the most utilized method to solve the field equation [22–27].

In the previously outlined framework, major problems involved in the micro scale computational modeling are: *i*) meshing curved objects i.e. fibre/matrix interfaces within a random-generated domain which can present geometrical difficulties or singularities (i.e. nearly touching objects); *ii*) efficient domain discretization for any realization and any given loading condition; *iii*) high computational cost due to a large number of realizations needed in a statistical homogenization process for it to accurately reach convergence.

Recently, the Virtual Element Method (VEM) has been proposed and shown to be a very efficient alternative to the standard finite element method [28,29]. It represents a generalization of the FE method with the capability of dealing with very general polygonal/polyhedral meshes. The VEM has already been successfully adopted to solve linear elasticity problems [30–32], as well as in conjunction with topology optimization and with complex material nonlinearity such as plasticity, viscoelasticity, damage and shape memory problems, see, e.g. Ref. [33–39] for a short representative list of related works. In the framework of computational homogenization, a VEM based procedure has been proposed in Ref. [20], for evaluating the antiplane shear homogenized material moduli of a doubly periodic composite material reinforced by cylindrical inclusions, more recently a study of particle-based composites via VEM has been presented in Refs. [18,19], adopting polygonal meshes for the matrix and a single element for the inclusions. An investigation on the capability and advantages of the VEM technique in solving the micromechanical and homogenization problem for periodic composites characterized by linear mechanical response has been performed in Ref. [40].

The aim of this communication is to develop a VEM based procedure for the antiplane shear homogenization problem which tackles and solves the above mentioned issues inherent to a numerical approach for the micromechanical problem, by making use of specific features of the virtual technology, namely the possibility of using curvilinear polygonal elements [41,42] (thus avoiding geometry discretization errors at fibre/matrix interface) and of using adaptive mesh refinement in order to get large scale analysis on several domain realizations with a reduced computational cost by tuning the mesh discretization through an ad-hoc a posteriori error estimator for the specific micromechanical problem under consideration. In particular, VEM elements characterized by linear and higher order polynomial approximation are proposed. Homogeneous and functionally graded constitutive laws are considered for the fibre constituents of the composite. Numerical applications are developed to assess the effectiveness of the proposed VEM elements by making several comparisons with results obtained adopting available more established techniques showing the advantages of the newly proposed methodology with respect to standard mesh generation and uniform refinement techniques.

The paper is organized as follows. In Section 2 the asymptotic homogenization problem under investigation is sketched for the case of long fibre composites. In Section 3 the curvilinear VEM formulation is described. Section 4 illustrates an a posteriori error estimator for the model under investigation together with its theoretical assessment and inherent adaptive mesh refinement capability. Section 5 presents a large class of numerical tests validating the curvilinear VEM and proving the effectiveness of the proposed method as a tool for the computational homogenization of random fibre reinforced materials. Finally, conclusive remarks are given in Section 6.

2. Asymptotic homogenization of random fibre-reinforced composite

We consider a composite material, reinforced with long, parallel fibres, randomly distributed in the material with a statistically homogeneous microstructure. Fibres have circular cross section and the same radius.

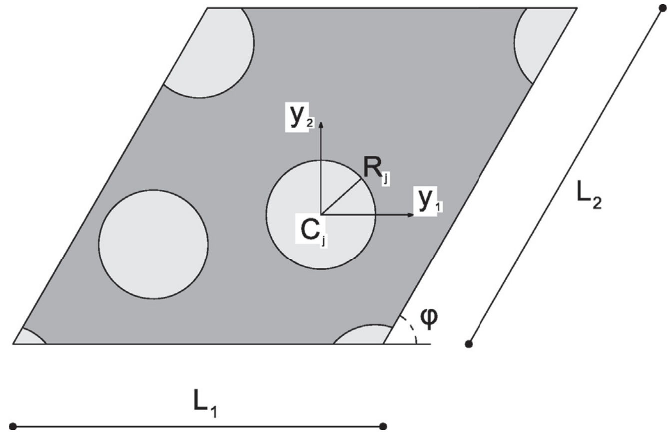

Fig. 1. A stochastic realization of a parallelogram shaped repeating unit cell (RUC) of the composite with volume fraction $f = 0.2$ and three circular fibres. Geometrical parameters and fibre frame reference.

At the microscale, the cross section of the composite consists of a doubly-periodic arrangement of repeating unit cells (RUC). Geometry-wise a RUC is a parallelogram, with sides L_1, L_2, and angle ϕ, containing the centres of F fibres, denoted by C_j, with radii R_j, $j = 1 \dots F$, as represented in Fig. 1. In the following, we will denote $f_j = \pi R_j^2/|\mathrm{D}|$ as the volume fraction of the jth fibre, and $f = \sum_{j=1}^{F} f_j$ as the total volume fraction.

In this treatment, reference will be made to effective in-plane elastic shear moduli, computed applying asymptotic homogenization. Hence, a family of equilibrium boundary value problems, indexed by a parameter ϵ, for the longitudinal (i.e. orthogonal to fibre cross section plane) displacement field w_ϵ, is considered on the composite domain:

$$\mathrm{div}(\boldsymbol{G}\nabla w_\epsilon) = 0 \qquad \text{in } \cup_j \Omega^{\mathrm{f}}_{j\epsilon} \cup \Omega^{\mathrm{m}}_{\epsilon}\,; \tag{1}$$

$$[[\boldsymbol{G}\nabla w_\epsilon \cdot \boldsymbol{v}]] = 0 \qquad \text{on } \cup_{\mathrm{j}} \Gamma_{\mathrm{j}\epsilon}\,; \tag{2}$$

$$\boldsymbol{G}\nabla w_\epsilon \cdot \boldsymbol{v} = \frac{1}{\epsilon} D_j [[w_\epsilon]] \qquad \text{on } \cup_{\mathrm{j}} \Gamma_{\mathrm{j}\epsilon}\,. \tag{3}$$

where $\cup_j \Omega^{\mathrm{f}}_{j\epsilon}$ and $\Omega^{\mathrm{m}}_{\epsilon}$ denote fibres and matrix domains respectively, $\cup_j \Gamma_{j\epsilon}$ is the set formed by fibre/matrix interfaces, $\boldsymbol{v}$ is unit vector normal to $\cup_j \Gamma_{j\epsilon}$ pointing into $\Omega^{\mathrm{m}}_{\epsilon}$, and square brackets $[[\cdot]]$ denote jump across the interface, defined as extra-fibre value minus intra-fibre value. In the above, the parameter ϵ scales the microstructure, such that $\epsilon = 1$ refers to the real composite material under consideration, and the homogenization limit is obtained by sending ϵ to zero.

Equation (1) is the field equilibrium equation; Eq. (3) represents equilibrium at the fibre/matrix interface requiring continuity of the normal-to-interface component of the shear stress; Eq. (2) is the interface constitutive law.

Assuming linear elastic fibres and matrix, the relative shear moduli are given by the constitutive tensor $\boldsymbol{G}$, which respectively reads:

$$\boldsymbol{G} = \boldsymbol{G}^{\mathrm{f}}_j \quad \text{in } \Omega^{\mathrm{f}}_{j\epsilon} \;\; j = 1 \dots F \tag{4}$$

$$\boldsymbol{G} = \boldsymbol{G}^{\mathrm{m}} \quad \text{in } \Omega^{\mathrm{m}}_{\epsilon}. \tag{5}$$

Fibres are made of a linear elastic material with cylindrical orthotropy, their material moduli are graded along the radius, such that, setting a polar coordinate system (C_j, r_j, θ_j) for each fibre, it results:

$$\boldsymbol{G}^{\mathrm{f}}_j = (G^{\mathrm{r}}_j \boldsymbol{e}^{\mathrm{r}}_j \otimes \boldsymbol{e}^{\mathrm{r}}_j + G^{\theta}_j \boldsymbol{e}^{\theta}_j \otimes \boldsymbol{e}^{\theta}_j) g_j(\rho_j), \tag{6}$$

where $\rho_j = r_j/R_j$, $g_j(\rho_j)$ is the grading function, and $(\boldsymbol{e}^{\mathrm{r}}_j, \boldsymbol{e}^{\theta}_j)$ are the radial and tangential unit vectors, respectively. The matrix material is homogeneous and isotropic, so that $\boldsymbol{G}^{\mathrm{m}} = G^{\mathrm{m}} I$, with I the second order identity tensor and G^{m} the matrix shear modulus.

Zero-thickness imperfect fibre/matrix interfaces are assumed according to the classical linear spring-layer model [11,43,44]. As can be deduced by Eq. (2), a linear elastic relation for the displacement jump $[[w_\varepsilon]]$ and the interface normal traction $\boldsymbol{G}\nabla w_\varepsilon \cdot \boldsymbol{\nu}$ is assumed through the parameter D_j, with the factor ε^{-1} granting the right scaling in the homogenization limit [11].

In order to guarantee the well posedness of the above problem, the following limitations hold true:

$$G^{\mathrm{m}} > 0 \quad G^{\mathrm{r}}_j > 0 \quad G^{\theta}_j > 0 \quad D_j > 0 \quad g_j(\rho_j) > 0 \quad \text{in } (0,1) \qquad j = 1 \ldots F. \tag{7}$$

2.1. Homogenized equilibrium equation

The asymptotic homogenization method is employed to derive the homogenized or effective constitutive tensor of the composite material. Two different length scales characterize the problem under consideration. Hence, two different space variables are introduced: the macroscopic one, x, and the microscopic one, $y = x/\varepsilon$, $y \in \mathsf{D}$, being D the RUC (see Fig. 1), whose extra-fibre space, intra-fibre space and fibre-matrix interface are denoted by D^{m}, $\mathsf{D}^{\mathrm{f}}_j$ and Γ_j, for $j = 1 \ldots F$, respectively. An asymptotic expansion of the unknown displacement field is considered in the form:

$$w_\varepsilon(x,y) = w_0(x,y) + \varepsilon w_1(x,y) + \varepsilon^2 w_2(x,y) + \ldots, \tag{8}$$

where w_0, w_1, w_2 are D-periodic functions in y, and w_1, w_2 have null integral average over D. Substituting (8) into Problem (1)–(2) and equating the power-like terms of ε, three differential problems for w_0, w_1 and w_2 are obtained, respectively, which, following a standard argument [6,9], yield the homogenized equation for the macroscopic displacement w_0:

$$\mathrm{div}_x(\boldsymbol{G}^{\#}\nabla_x w_0) = 0. \tag{9}$$

Here $\nabla_x w_0$ is the macroscopic shear strain, and

$$\boldsymbol{G}^{\#} = \frac{1}{|\mathsf{D}|}\int_{\mathsf{D}} \boldsymbol{G}\left(I - \nabla^{\mathrm{t}}_y \chi\right)\,\mathrm{d}a \tag{10}$$

is the effective constitutive tensor, where the superscript $^{\mathrm{t}}$ denotes the transpose, da is the area element of D, $|\cdot|$ is the Lebesgue measure, and the vector-valued cell function $\chi(y)$ has been introduced. Its components $\chi_s, s = 1, 2$, are the unique, null average, D-periodic solutions of the cell problem:

$$\mathrm{div}_y[\boldsymbol{G}(\nabla_y\chi_s - \boldsymbol{e}_s)] = 0 \qquad \text{in } \mathsf{D}^{\mathrm{f}} \cup \mathsf{D}^{\mathrm{m}}\,; \tag{11}$$

$$[[\boldsymbol{G}(\nabla_y\chi_s - \boldsymbol{e}_s)\cdot\boldsymbol{\nu}]] = 0 \qquad \text{on } \cup_{\mathrm{j}}\Gamma_{\mathrm{j}}\,; \tag{12}$$

$$\boldsymbol{G}(\nabla_y\chi_s - \boldsymbol{e}_s)\cdot\boldsymbol{\nu} = D_j[[\chi_s]] \qquad \text{on } \cup_{\mathrm{j}}\Gamma_{\mathrm{j}} \tag{13}$$

where $\boldsymbol{e}_s$ is the unit vector parallel to the y_s axis.

Using the Gauss-Green Lemma and introducing the auxiliary cell function:

$$\widetilde{\chi}(y_1,y_2) = \chi(y_1,y_2) - (y_1\boldsymbol{e}_1 + y_2\boldsymbol{e}_2), \tag{14}$$

Eq. (10) is transformed into:

$$\boldsymbol{G}^{\#} = \boldsymbol{G}^{\mathrm{m}} + \frac{1}{|\mathsf{D}|}\sum_{j=1}^{F}\int_{\mathsf{D}^{\mathrm{f}}_j}(\mathrm{div}_y\boldsymbol{G}^{\mathrm{f}})\otimes\widetilde{\chi}\,\mathrm{d}a + \frac{1}{|\mathsf{D}|}\sum_{j=1}^{F}\int_{\Gamma_j}[[\boldsymbol{G}\boldsymbol{\nu}\otimes\widetilde{\chi}]]\,\mathrm{d}l, \tag{15}$$

where dl is the line element of Γ_j. Equation (15) yields the effective shear moduli of the composite material in terms of the solution χ of the cell problem.

3. C^0 curved virtual element method

A weak formulation for the cell problem (11)-(13) is provided by the virtual work principle:

$$\begin{cases} \text{Find } \widetilde{\chi}_s \in \widetilde{V} \text{ such that} \\ a(\widetilde{\chi}_s, \delta\chi_s) = 0 \quad \forall\,\delta\chi_s \in V,\ s = 1,2 \end{cases} \tag{16}$$

where $\widetilde{V} := H^1_{sp}(\mathsf{D})$ is the space of the admissible auxiliary cell functions $\widetilde{\chi}$ which are shift D-periodic, i.e. such that the associated $\chi_s(y_1,y_2)$ function (that is, the corresponding component s of the vector field in (14)) satisfies

$$\chi_s(y_1 + L_1, y_2) = \chi_s(y_1,y_2) = \chi_s(y_1 + L_2\cos\phi, y_2 + L_2\sin\phi). \tag{17}$$

More precisely ($s \in \{1,2\}$)

$$\widetilde{V} = \{\widetilde{\chi} \in L^2(\mathsf{D}) \text{ such that } \widetilde{\chi}\,|_{\mathsf{D}^{\mathrm{f}}_j} \in H^1(\mathsf{D}^{\mathrm{f}}_j) \text{ for } j = 1,2,..,F,$$
$$\widetilde{\chi}\,|_{\mathsf{D}^{\mathrm{m}}} \in H^1(\mathsf{D}^{\mathrm{m}}),\ \widetilde{\chi}(y_1,y_2) + y_s \text{ satisfies (17)}\}.$$

Note that, due to the last condition, the space $\widetilde{V}$ depends on $s \in \{1,2\}$, but we prefer to avoid expliciting such dependence in the notation. We denote by V the space of the admissible D-periodic variations of $\widetilde{V}$. The bilinear form characterizing the variational formulation is:

$$a(\widetilde{\chi}_s, \delta\chi_s) = -\int_{\mathsf{D}} \mathrm{div}_y[\boldsymbol{G}(\nabla_y\widetilde{\chi}_s)]\,\delta\chi_s\,dx \tag{18}$$

which, exploiting Gauss-Green lemma, considering constitutive equation (13) and that unit normal vectors to $\partial\mathsf{D}^{\mathrm{m}}$ on opposite sides of the unit cell are opposite, becomes:

$$a(\widetilde{\chi}_s, \delta\chi_s) = \int_{\mathsf{D}^{\mathrm{m}}}\nabla_y\delta\chi_s \cdot \boldsymbol{G}^{\mathrm{m}}(\nabla_y\widetilde{\chi}_s)dx + \sum_{j=1}^{F}\int_{\mathsf{D}^{\mathrm{f}}_j}\nabla_y\delta\chi_s \cdot \boldsymbol{G}^{\mathrm{f}}_j(\nabla_y\widetilde{\chi}_s)dx + \sum_{j=1}^{F}\int_{\Gamma_j}[[\delta\chi_s]]\,D_j\,[[\widetilde{\chi}_s]]\,dl. \tag{19}$$

In more compact notation, one can also write

$$a(\widetilde{\chi}_s, \delta\chi_s) = \int_{\mathsf{D}}\nabla_y\delta\chi_s \cdot \boldsymbol{G}(\nabla_y\widetilde{\chi}_s)dx + \sum_{j=1}^{F}\int_{\Gamma_j}[[\delta\chi_s]]\,D_j\,[[\widetilde{\chi}_s]]\,dl. \tag{20}$$

The form $a(\cdot,\cdot)$ is symmetric, continuous and coercive on $\widetilde{V}$, so that problem (16) is well posed.

3.1. The virtual element space

Aiming at a virtual element discretization of problem (16) with curved edges, we follow the same lines of [41]. Let $\boldsymbol{\mathcal{T}}_h$ be a *simple polygonal mesh* on D, i.e. any decomposition of D in a finite set of simple polygons E, without holes and with boundary given by a finite number of edges. Whenever an element has an edge lying on an interface Γ_j, such edge is then allowed to be curved in order to describe exactly the geometry of the problem. We assume that each interface Γ_j is parametrized by an invertible C^1 mapping γ_j from an interval in the real line into Γ_j. It is not restrictive to assume that each curved edge is a subset of only one Γ_j and therefore regular. In order to simplify the notation in the following we sometimes drop the index j, simply use Γ and

$$\boldsymbol{\gamma} : [0,L] \Longrightarrow \Gamma$$

to indicate a generic curved part of the fibre/matrix interface and its associated parametrization.

In the following we will denote with e a generic edge of the mesh and with v a generic vertex. As usual the symbol h will be associated to the diameter of objects, for instance h_E will denote the diameter of the element E and h_e the (curvilinear) length of the edge e. An h without indexes denotes as usual the maximum mesh element size.

3.2. The virtual space

In the present section we briefly review the space proposed in Ref. [41], that we will use for the discretization of the problem. As usual, we define the space element by element. Let therefore $E \in \mathcal{T}_h$. Note that E may have some curved edge, laying on some curved interface Γ_j ($j \in \{1,2,..,F\}$). For any of such curved edges e, let $\boldsymbol{\gamma}_e : [a,b] \to e$ denote the restriction of the parametrization describing Γ_j to the edge e. Then we indicate the space of mapped polynomials (living on e) as

$$\widetilde{\mathcal{P}}_k(e) = \{p \circ \boldsymbol{\gamma}_e^{-1} : p \in \mathcal{P}_k[a,b]\}.$$

The local virtual element space on E is then defined as

$$\begin{aligned} V_h(E) =\{&v \in H^1(E) \cap C^0(E) : v\,|_e \in \mathcal{P}_k(e) \text{ if } e \text{ is straight}, \\ &v\,|_e \in \widetilde{\mathcal{P}}_k(e) \text{ if } e \text{ is curved}, -\Delta v \in \mathcal{P}_{k-2}(E)\}. \end{aligned} \tag{21}$$

The associated degrees of freedom are (see Ref. [41] for the simple Proof).

- pointwise evaluation at each vertex of E;
- pointwise evaluation at $k-1$ distinct points for each edge of E;
- moments $\int_E v p_{k-2}$ for all $p_{k-2} \in \mathcal{P}_{k-2}(E)$.

As usual, the global space is obtained by a standard gluing procedure

$$\widetilde{V}_h = \{v \in \widetilde{V} : v\,|_E \in V_h(E)\ \forall E \in \mathcal{T}_h\},$$

and the same holds for the corresponding space of discrete variations

$$V_h = \{v \in V : v\,|_E \in V_h(E)\ \forall E \in \mathcal{T}_h\}.$$

The global degrees of freeedom are the obvious extension of the local ones. Note that on the edges of the mesh the degrees of freedom are standard Lagrange type interpolation points. Therefore, handling the discontinuities across interfaces and the periodic boundary conditions in the definition of $H^1_{sp}(\mathrm{D})$ is done exactly as in standard finite elements.

3.3. Discretization of the problem

The discretization of the problem is a combination of the scheme proposed in Ref. [20] for the case with standard straight edges and the curved-edge technology introduced in Ref. [41] for a model linear diffusion problem.

We start by introducing the following projection operator that is used to compute, on each mesh element E, an approximated gradient operator. Let $[\mathcal{P}_{k-1}(E)]^2$ denote the set of polynomial vector fields of degree $k-1$ living on E. Given $E \in \mathcal{T}_h$ and any $v_h \in V_h(E)$, the operator $\Pi : V_h(E) \to [\mathcal{P}_{k-1}(E)]^2$ is defined by

$$\begin{cases} \Pi(v_h) \in [\mathcal{P}_{k-1}(E)]^2 \\ \displaystyle\int_E \Pi(v_h) \cdot \mathbf{p}_{k-1} = \int_E \nabla(v_h) \cdot \mathbf{p}_{k-1} \quad \forall \mathbf{p}_{k-1} \in [\mathcal{P}_{k-1}(E)]^2, \end{cases}$$

where $\nabla(v_h)$ denotes as usual the gradient of v_h (we dropped the y to simplify the notation). By definition, $\Pi(v_h)$ is the L^2 projection of ∇v_h on $[\mathcal{P}_{k-1}(E)]^2$. Note that the above operator is computable. Indeed an integration by parts shows that

$$\int_E \nabla v_h \cdot \mathbf{p}_{k-1} = -\int_E v_h(\mathrm{div}\,\mathbf{p}_{k-1}) + \int_{\partial E} v_h(\mathbf{p}_{k-1}\mathbf{n}_E).$$

The first term on the right hand side can be computed noting that $\mathrm{div}\mathbf{p}_{k-1}$ is a polynomial of degree $k-2$ and using the internal degrees of freedom values of v_h. The second term on the right hand side can be computed since we have complete knowledge of v_h on the boundary of E. Note that all these computations clearly require the integration of known functions on a curved element and a curved boundary; those can be accomplished as shown for instance in Ref. [41,45,46].

We can now describe the proposed numerical method. We start by defining the local discrete counterpart of the first bilinear form appearing in the right hand side of (20). Let $E \in \mathcal{T}_h$. We define for all $v_h, w_h \in V_h(E)$ the local discrete bilinear form as

$$a_h^E(v_h, w_h) = \int_E \Pi w_h \cdot \boldsymbol{G}(\Pi v_h)\,dx + s^E((I-\pi)v_h, (I-\pi)w_h) \tag{22}$$

where the first term is a direct approximation of $\int_E \nabla w_h \cdot \boldsymbol{G}(\nabla v_h)$ by substituting ∇ with Π, and the second term is the stabilization form, described below. The operator $\pi : V_h(E) \to \mathcal{P}_k(E)$ can be chosen as any projection operator on polynomials of degree k, for instance one that minimizes the distance of the euclidean norm of the degree of freedom values (such particular choice has the advantage of being very simple to code, see for instance Refs. [32]). The stabilization form can be taken, for example, as

$$s^E((I-\pi)v_h, (I-\pi)w_h) = \alpha_E \sum_{i=1}^{\#dofs} (dof_i(w_h - \pi w_h))\,(dof_i(v_h - \pi v_h)) \tag{23}$$

where the dof_i symbol denotes evaluation at the ith local degree of freedom and the positive scalar α_E is introduced in order to take into account the material constants. For example one can take $\alpha_E = \mathrm{trace}(\boldsymbol{G}(\mathbf{x}_E))/2$ with $\mathbf{x}_E$ the centroid of E or any other internal point (the method turns out to be quite robust with respect to this parameter). Note that the above stabilization, that is quite awkward to write on paper, is instead very simple to code since it is directly based on the degree of freedom values, that is what the code operates on. More details on the stabilization can be found for instance in Refs. [32].

The global discrete bilinear form is now taken as, for any v_h, w_h in $\widetilde{V}_h$ or V_h,

$$a_h(v_h, w_h) = \sum_{E \in \mathcal{T}_h} a_h^E(v_h, w_h) + \sum_{j=1}^{F} \int_{\Gamma_j} [\![w_h]\!]\, D_j\, [\![v_h]\!]\, dl$$

where we observe that the jumps above can be immediately computed since the virtual functions are known explicitly on the boundaries of the elements.

The proposed Virtual Element Method then reads

$$\begin{cases} \text{Find } \widetilde{\chi}_{hs} \in \widetilde{\mathrm{V}}_h \text{ such that} \\ a_h(\widetilde{\chi}_{hs}, \delta\chi_{hs}) = 0 \qquad \forall \delta\chi_{hs} \in \mathrm{V}_h,\ s = 1,2. \end{cases} \tag{24}$$

To ease notation, in the following, we simply indicate either component $\chi_{hs}, s = 1,2$ of the cell function with χ_h, explicitly indicating a specific component whenever needed. Note that the above construction follows the same logic and structure as for the straight-edge case [20,28] and we refer to such papers for a more detailed description of the practical implementation of the scheme. In the code, the main difference is only the need to integrate along curved edges and on curved domains (that can be handled following the literature given above).

4. A posteriori error estimator

In the present section, inspired by Ref. [47] (see also [48]) we introduce the proposed error estimator, and develop a theoretical reliability analysis (i.e. the estimator bounds the error from above) that takes into account the material constants appearing in the problem.

We start by introducing some notation. In the following we assume for simplicity that the material tensor $\boldsymbol{G}$ is piecewise constant with respect to the mesh (see also Remark 4.1), and we define for each element $E \in \mathcal{T}_h$ the positive constants $G_E^{inf}, G_E^{\sup}$ by

$$G_E^{inf} \le \frac{\mathbf{w} \cdot \boldsymbol{G}\,|_E \mathbf{w}}{\mathbf{w} \cdot \mathbf{w}} \le G_E^{\sup} \quad \forall \mathbf{w} \in \mathbb{R}^2. \tag{25}$$

Moreover for each internal edge e, denoting by $E^{\pm}$ the two elements sharing e, we define

$$G_e^{inf} := \min\{G_{E^+}^{inf}, G_{E^-}^{inf}\}.$$

In order to simplify the notation, we introduce an additional assumption, which controls the jumps of $\boldsymbol{G}$ among adjacent elements of the same subdomain. Given any element E, let ω_E denote the union of all elements sharing at least a vertex with E and that lay in the same subdomain as E (either $\mathsf{D}_j^{\mathsf{f}}$ for some index j or D^{m}). Then, there exist two constants $c_\star, c^\star$ such that for all $E \in \mathcal{T}_h$ it holds

$$c_\star G_{E'}^{inf} \le G_E^{inf} \le c^\star G_{E'}^{inf} \qquad \forall E' \in \omega_E, \tag{26}$$

and the analogous for $G_E^{\sup}$.

Given $\widetilde{\chi}_h$ solution to the discrete problem (24), we introduce the following terms for the error indicator. For each $E \in \mathcal{T}_h$ we define the internal residual term

$$\eta_{R,E}^2 := \frac{h_E^2}{G_E^{inf}} \|\mathrm{div}_y[\boldsymbol{G}(\Pi\,\widetilde{\chi}_h)]\|_{L^2(E)}^2.$$

For each edge e of the mesh, including the boundary and interface ones, we define the edge residual term

$$\eta_{r,e}^2 := \frac{h_e}{G_e^{inf}} \|\,[[\boldsymbol{G}(\Pi\,\widetilde{\chi}_h)\cdot \boldsymbol{v}_e]]\,\|_{L^2(e)}^2.$$

For each edge e on the interface Γ we also consider the interface residual term

$$\eta_{\Gamma,e}^2 := \frac{h_e}{G_e^{inf}} \|\,\{\boldsymbol{G}(\Pi\,\widetilde{\chi}_h)\cdot \boldsymbol{v}_e\} - D[[\chi_h]]\,\|_{L^2(e)}^2,$$

where the $\{\dots\}$ symbol above denotes the average operator among the left and right elements sharing the edge e. Furthermore, for each element $E \in \mathcal{T}_h$ we consider the additional term taking into account the inconsistency stemming from the VEM formulation

$$\eta_{S,E}^2 := s^E((I-\pi)\widetilde{\chi}_h, (I-\pi)\widetilde{\chi}_h).$$

Finally, the local and global error estimators are

$$\eta_E^2 = \eta_{R,E}^2 + \eta_{S,E}^2 + \frac{1}{2}\sum_{e\in\partial E}\eta_{r,e}^2 + \frac{1}{2}\sum_{e\in\partial E\cap\Gamma}\eta_{\Gamma,e}^2 \qquad \forall E \in \mathcal{T}_h, \tag{27}$$

$$\eta^2 = \sum_{E\in\mathcal{T}_h}\eta_E^2. \tag{28}$$

In the following we assume that the operator π in (23) is continuous in the H^1 norm, a property that holds for essentially all choices used in the literature. In order to state the reliability result we require the following mesh assumptions, that are standard in the VEM literature.

Mesh assumptions. There exists a positive constant ρ such that all elements E of the mesh family $\{\mathcal{T}_h\}_h$ are star-shaped with respect to a ball with radius $R_E \ge \rho h_E$. Moreover all edges e of each element E of the mesh family $\{\mathcal{T}_h\}_h$ have length $h_e \ge \rho h_E$.

Theorem 4.1. *Let the mesh assumptions above hold. Then it exists a uniform constant C, independent of the mesh and the material constants, such that the error $\widetilde{\chi} - \widetilde{\chi}_h$ satisfies*

$$a(\widetilde{\chi} - \widetilde{\chi}_h, \widetilde{\chi} - \widetilde{\chi}_h) \le C\,\eta^2.$$

Proof. In the following the symbol $\lesssim$ will denote a bound up to a constant that is independent of the mesh and the material constants. We note that the constant $\alpha_E = \mathrm{trace}(\boldsymbol{G}(x_E))/2$ proposed for the stabilization term in (23) is equivalent (up to universal constants) to $G_E^{\sup}$. Therefore, assuming to use stabilization (23) and recalling standard results in the VEM literature (see, e.g. Refs. [29,49]), we have for all elements E and all v_h in the discrete space

$$\begin{aligned} G_E^{\sup}\|\nabla(I-\pi)v_h\|_{L^2(E)}^2 &\lesssim s^E((I-\pi)v_h, (I-\pi)v_h) \\ &\lesssim G_E^{\sup}\|\nabla(I-\pi)v_h\|_{L^2(E)}^2. \end{aligned} \tag{29}$$

Let the error $\phi = \widetilde{\chi} - \widetilde{\chi}_h \in V$ and let $\phi_I \in V_h$ be an interpolant of ϕ to be better defined later. First using the continuous equation (16), then adding/subtracting ϕ_I and using (24), we obtain

$$\begin{aligned} a(\widetilde{\chi} - \widetilde{\chi}_h, \widetilde{\chi} - \widetilde{\chi}_h) &= a(\widetilde{\chi} - \widetilde{\chi}_h, \phi) = -a(\widetilde{\chi}_h, \phi) \\ &= -a(\widetilde{\chi}_h, \phi - \phi_I) - a(\widetilde{\chi}_h, \phi_I) \\ &= -a(\widetilde{\chi}_h, \phi - \phi_I) - a(\widetilde{\chi}_h, \phi_I) + a_h(\widetilde{\chi}_h, \phi_I). \end{aligned} \tag{30}$$

By recalling that $\Pi\widetilde{\chi}_h$ is the L^2 projection of $\nabla\widetilde{\chi}_h$ on $[\mathcal{P}_{k-1}(E)]^2$ and noting that $\nabla\pi\widetilde{\chi}_h \in [\mathcal{P}_{k-1}(E)]^2$, we can derive the following preliminary bounds for all elements E

$$\begin{aligned} &\|\boldsymbol{G}^{1/2}(\nabla\widetilde{\chi}_h - \Pi\widetilde{\chi}_h)\|_{L^2(E)}^2 \le G_E^{\sup}\|\nabla\widetilde{\chi}_h - \Pi\widetilde{\chi}_h\|_{L^2(E)}^2 \\ &\le G_E^{\sup}\|\nabla\widetilde{\chi}_h - \nabla\pi\widetilde{\chi}_h\|_{L^2(E)}^2 \lesssim s^E((I-\pi)\widetilde{\chi}_h, ((I-\pi)\widetilde{\chi}_h), \end{aligned} \tag{31}$$

where we used (29). Let us observe that it holds

$$\begin{aligned} a(\widetilde{\chi}_h, \phi - \phi_I) &= \sum_{E\in\mathcal{T}_h}\int_E (\nabla\widetilde{\chi}_h - \Pi\widetilde{\chi}_h)\cdot\boldsymbol{G}\nabla(\phi-\phi_I)dx \\ &\quad + \sum_{E\in\mathcal{T}_h}\int_E \Pi\widetilde{\chi}_h\cdot\boldsymbol{G}\nabla(\phi-\phi_I)dx \\ &\quad + \sum_{j=1}^{F}\int_{\Gamma_j}[[\widetilde{\chi}_h]]D_j[[\phi-\phi_I]]dl \\ &= \sum_{E\in\mathcal{T}_h}(I_E + II_E) + \sum_{j=1}^{F}\int_{\Gamma_j}[[\widetilde{\chi}_h]]D_j[[\phi-\phi_I]]dl. \end{aligned}$$

Employing the Cauchy-Schwarz inequality, (25) and (31) we obtain

$$\begin{aligned} \sum_{E\in\mathcal{T}_h} I_E &\lesssim \left(\sum_{E\in\mathcal{T}_h} s^E((I-\pi)\widetilde{\chi}_h, (I-\pi)\widetilde{\chi}_h)\right)^{1/2} \\ &\quad \left(\sum_{E\in\mathcal{T}_h} G_E^{\sup}\|\nabla(\phi-\phi_I)\|_{L^2(E)}^2\right)^{1/2}. \end{aligned}$$

Moreover, integration by parts yields

$$\begin{aligned} \sum_{E\in\mathcal{T}_h} II_E &= -\sum_{E\in\mathcal{T}_h}\int_E \nabla\cdot(\boldsymbol{G}\Pi\widetilde{\chi}_h)(\phi-\phi_I)dx \\ &\quad - \sum_{e\in\mathcal{E}_h}\int_e [[\boldsymbol{G}\Pi\widetilde{\chi}_h\cdot\boldsymbol{v}_e]]\{\phi-\phi_I\}dl \\ &\quad - \sum_{j=1}^{F}\sum_{e\in\Gamma_j}\int_e \{\boldsymbol{G}\Pi\widetilde{\chi}_h\cdot\boldsymbol{v}_e\}[[\phi-\phi_I]]. \end{aligned}$$

Secondly, first recalling the definition of Π and that $\boldsymbol{G}\,|_E$ is constant, then using again (31) and standard properties of symmetric bilinear forms we have

$$\begin{aligned} &a_h(\widetilde{\chi}_h, \phi_I) - a(\widetilde{\chi}_h, \phi_I) \\ &= \sum_{E\in\mathcal{T}_h}\left(\int_E (\Pi\widetilde{\chi}_h - \nabla\widetilde{\chi}_h)\cdot\boldsymbol{G}\nabla\phi_I dx + s^E((I-\pi)\widetilde{\chi}_h, (I-\pi)\phi_I)\right) \\ &\lesssim \left(\sum_{E\in\mathcal{T}_h} s^E((I-\pi)\widetilde{\chi}_h, (I-\pi)\widetilde{\chi}_h)\right)^{1/2} \\ &\left(\sum_{E\in\mathcal{T}_h}\|\boldsymbol{G}^{1/2}\nabla\phi_I\|_{L^2(E)}^2 + s^E((I-\pi)\phi_I, (I-\pi)\phi_I)\right)^{1/2}. \end{aligned}$$

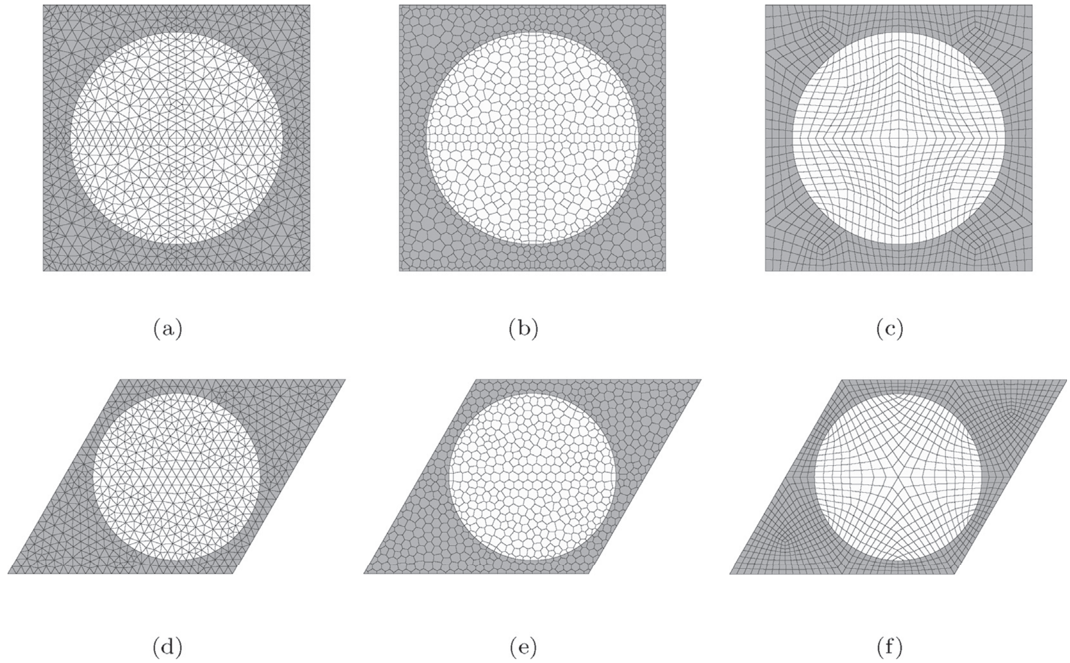

Fig. 2. Doubly periodic composite. Representative unit cell meshes. Upper row: square lattice; lower row: parallelogram lattice. Circular fibre inclusion with volume fraction $f = 0.5$. (a)–(d) Tri-mesh. (b)–(e) Poly-mesh. (c)–(f) Quad-mesh.

We now observe that (29) and the continuity of the operator π in H^1 yield

$$s^E((I-\pi)\phi_I,(I-\pi)\phi_I) \lessapprox G_E^{\sup}\|\nabla(I-\pi)\phi_I\|^2_{L^2(E)} \lessapprox G_E^{\sup}\|\nabla\phi_I\|^2_{L^2(E)}. \quad (32)$$

Collecting the above terms in (30), we obtain

$$\begin{aligned}
a(\phi,\phi) \lessapprox & \left(\sum_{E\in\mathcal{T}_h} s^E\left((I-\pi)\widetilde{\chi}_h,(I-\pi)\widetilde{\chi}_h\right)\right)^{1/2} \\
& \left(\sum_{E\in\mathcal{T}_h} G_E^{\sup}\|\nabla(\phi-\phi_I)\|^2_{L^2(E)}\right)^{1/2} \\
& + \sum_{j=1}^{F}\sum_{e\in\Gamma_j}\|\{\boldsymbol{G}\Pi\widetilde{\chi}_h\cdot\boldsymbol{\nu}_e\}-D_j[[\widetilde{\chi}_h]]\|_{L^2(e)}\|[[\phi-\phi_I]]\|_{L^2(e)} \\
& + \sum_{E\in\mathcal{T}_h}\|\nabla\cdot\left(\boldsymbol{G}\Pi\widetilde{\chi}_h\right)\|_{L^2(E)}\|\phi-\phi_I\|_{L^2(E)} \\
& + \sum_{e\in\mathcal{E}_h}\|[[\boldsymbol{G}\Pi\widetilde{\chi}_h\cdot\boldsymbol{\nu}_e]]\|_{L^2(e)}\|\{\phi-\phi_I\}\|_{L^2(e)} \\
& + \left(\sum_{E\in\mathcal{T}_h} s^E((I-\pi)\widetilde{\chi}_h,(I-\pi)\widetilde{\chi}_h)\right)^{1/2} \\
& \left(\sum_{E\in\mathcal{T}_h} G_E^{\sup}\|\nabla\phi_I\|^2_{L^2(E)}\right)^{1/2}. \quad (33)
\end{aligned}$$

We now select $\phi_I \in V_h$ (that we define piecewise on each $\mathsf{D}_j^{\mathrm{f}}$ or D^{m} and therefore may have jumps across the subdomains) as the Clément-type interpolant operator for the Virtual Elements introduced in Ref. [50], here extended in trivial way to the case with curved edges. By combining the theoretical results in Ref. [50] with those derived in Ref. [41] for curved edges, one can obtain the following approximation results for all elements E (and $e \in \partial E$)

$$\|\phi-\phi_I\|_{L^2(E)} \lessapprox h_E\|\nabla\phi\|_{L^2(\omega_E)}$$

$$\|\nabla\phi_I\|_{L^2(E)} \leq \|\nabla\phi\|_{L^2(\omega_E)}$$

$$\|(\phi-\phi_I)\,|_E\|_{L^2(e)} \lessapprox h_E^{1/2}\|\nabla\phi\|_{L^2(\omega_E)} \quad (34)$$

where ω_E denotes the union of all elements sharing at least a vertex with E and that lay in the same subdomain as E (either $\mathsf{D}_j^{\mathrm{f}}$ for some index j or D^{m}).

Employing in (33) the above bounds together with standard trace inequalities, (25) and assumption (26) yields the thesis:

$$\begin{aligned}
a(\phi,\phi) \lessapprox & \sum_{E\in\mathcal{T}_h}\frac{h_E^2}{G_E^{inf}}\|\nabla\cdot(\boldsymbol{G}\Pi\widetilde{\chi}_h)\|^2_{L^2(E)} \\
& + \sum_{e\in\mathcal{E}_h}\frac{h_e}{G_e^{inf}}\|[[\boldsymbol{G}\Pi\widetilde{\chi}_h\cdot\boldsymbol{\nu}_e]]\|^2_{L^2(e)} \\
& + \sum_{j=1}^{F}\sum_{e\in F_j}\frac{h_e}{G_e^{inf}}\|\{\boldsymbol{G}\Pi\widetilde{\chi}_h\cdot\boldsymbol{\nu}_e\}-D_j[[\widetilde{\chi}_h]]\|^2_{L^2(e)} \\
& + \max_{E\in\mathcal{T}_h}(G_E^{\sup}/G_E^{inf})\sum_{E\in\mathcal{T}_h}s^E((I-\pi)\widetilde{\chi}_h,(I-\pi)\widetilde{\chi}_h.
\end{aligned}$$

Remark 4.1. *The assumption on the material tensor, i.e.* **G** *piecewise constant with respect to the mesh, can be relaxed. For instance,* Theorem 4.1 *is still valid with the same expression for the* a posteriori *error indicator* η *if we suppose that* **G** *is a smooth function on the computational mesh. However, suitable quadrature formulas have to be employed in order to practically compute the internal, boundary and interface residual terms. Moreover, the efficiency of the error indicators requires to control the so-called oscillation terms measuring the polynomial approximation of the tensor* **G** [51].

4.1. Adaptive curved virtual element method (ACVEM)

This section is devoted to describing how the above a-posteriori error estimate can be employed to drive an adaptive mesh refinement procedure. As detailed in the following section, adaptivity represents a crucial tool to efficiently compute overall elastic properties for random fibre reinforced composites. Similarly to, e.g. Refs. [52,53], we here

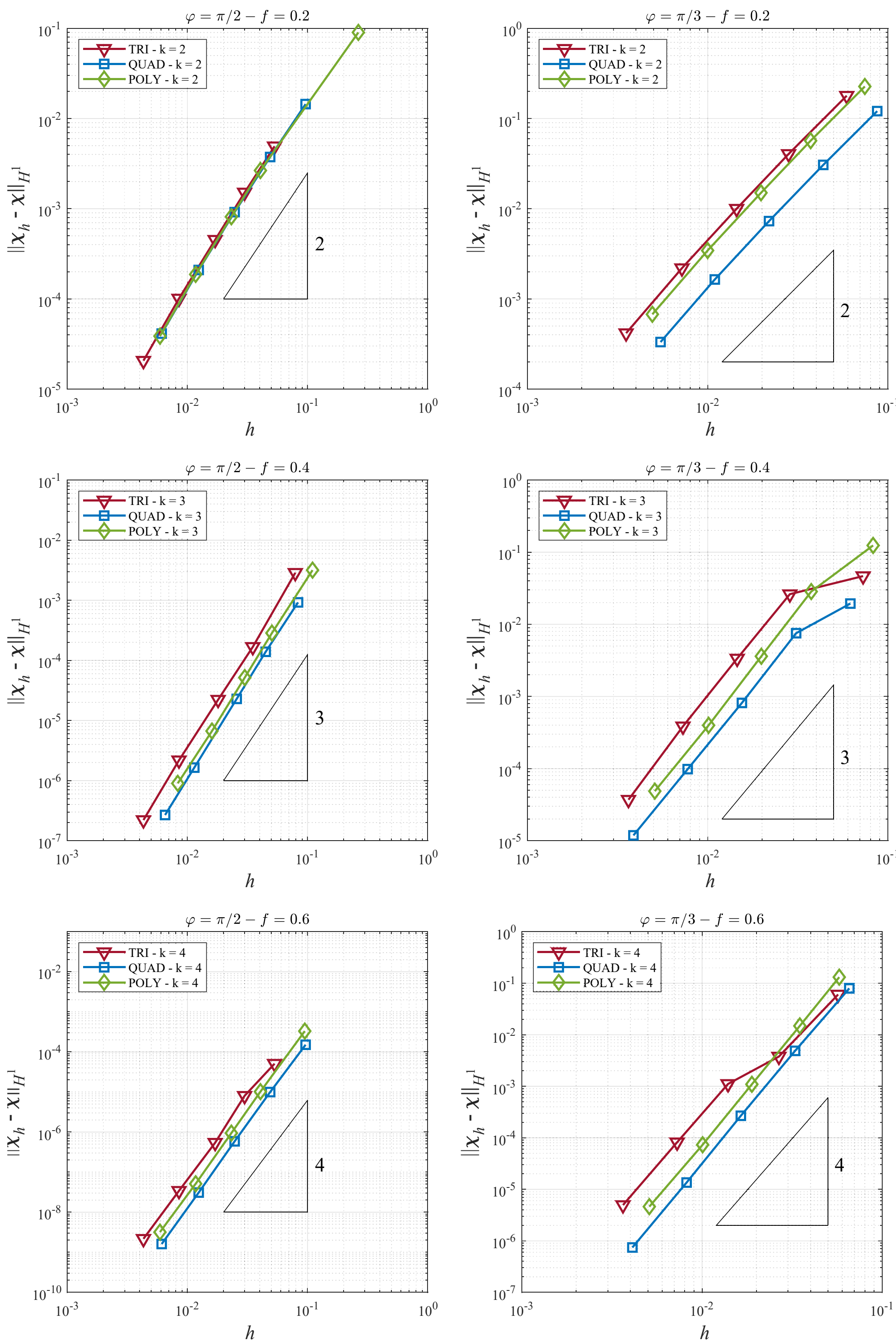

Fig. 3. Doubly periodic composites, with $f = 0.2, 0.4, 0.6$. $h-$convergence plots for $k = 2, 3, 4$, for the cell function $\chi(y)$ in the H^1-error norm for uniform mesh refinement. Left column: square lattice, isotropic homogeneous fibres: $\delta = \rightarrow \infty$, $\xi = 500$. Right column: parallelogram lattice, isotropic exponentially graded fibres: $\xi = 500, \omega = 8, \delta = 10$.

devise ACVEM based on the classical paradigm (see, e.g. Refs. [54], and the references therein):

SOLVE → ESTIMATE → MARK → REFINE

Staggered along the following steps. Given an initial (relatively coarse) representative unit cell mesh on which a solution has been computed:

- compute local element error indicators (see Eq. (27));
- sort elements with respect to local error indicator;
- mark elements according to the so-called Dörfler marking strategy, i.e. starting from the local largest error indicator and proceeding in a decreasing order mark the corresponding elements until a fixed percentage (here we employ 40%) of the global error indicator η is reached.
- refine marked elements adopting centroid-edge midpoint ray algorithm [52,53];
- compute a new solution for the refined mesh;
- iterate until a certain threshold for the global error is reached.

5. Numerical tests

This section presents numerical tests on the proposed VEM based strategy for the homogenization of fibre-reinforced composite materials. In particular, in Section 5.1 we numerically explore the accuracy and convergence properties of the curved virtual element method for the asymptotic homogenization in the basic case of doubly periodic composite materials adopting uniform mesh refinement. In Section 5.2, we apply the mesh refinement algorithm of Section 4.1 to investigate the capability of our a posteriori error estimate to drive an effective adaptive procedure. Last, in Section 5.3 we address statistical homogenization of composite materials with randomly distributed fibres by joint application of the adaptive mesh refinement strategy and Monte Carlo simulations.

5.1. Validation and accuracy of curved virtual element technology: doubly periodic functionally graded fibre reinforced composite

For accuracy and convergence assessment, we here study doubly periodic fibre reinforced composites for different fibre arrangements and material setups. A given doubly periodic composite unit cell is identified through the usual dimensionless geometrical parameters ϕ, $\kappa = L_2/L_1, f = \pi R^2/|\mathsf{D}|$ (being R the radius of the single circular fibre embedded into the RUC), and the following ones for material properties:

- fibre/matrix stiffness ratio (contrast factor) $\xi = G^{\mathrm{r}}/G^{\mathrm{m}}$;
- grading intensity factor $\omega = g(0)/g(1)$;
- dimensionless interface parameter $\delta = D/(G^{\mathrm{m}} L_1)$;
- $\sigma^2 = G^{\theta}/G^{\mathrm{r}}$.

The simulations refer to isotropic exponentially-graded fibres, with $g(\rho) = \exp(-\lambda\rho)$, and $\sigma = 1$, so that $g(0) = 1$, and $G^{\mathrm{r}} = G^{\theta}$ represents the shear modulus at fibre axis. We present results corresponding to three types of mesh discretizations, namely triangles, Voronoi polygons, quadrilaterals, indicated in the sequel as Tri-mesh, Poly-mesh, Quad-mesh, respectively. Representative meshes for square (resp. parallelogram) unit cell are portrayed in Fig. 2 with the three types of adopted discretizations. Presented results are obtained for order $k = 2, 3, 4$, respectively. As reference results we use the analytical method provided in Ref. [55] selecting a high number of terms in the series expansion for the unknown cell function in order to have high accuracy.

In Fig. 3 we report $h-$convergence plots for the cell function $\chi(y)$ in the H^1-error norm for uniform mesh refinement, for a set of cases selected as the more significant ones over an extensive test campaign.

Since the exact solution is piecewise regular in each subdomain and we have an exact geometric representation of the interface, the expected convergence rate is $O(h^k)$ (see Ref. [41]) which is obtained for all examined material patterns and any given order k. We notice that quadrilateral elements produce slightly more accurate results among the three compared discretizations. From a standpoint of material setup effect on overall accuracy, it is observed that skew unit cells as well as non-homogeneous fibres require higher computational cost to reach a given accuracy level with respect to homogeneous fibres lodged into a square lattice. As a further Proof of the efficiency of a curved element approach for the problem under investigation, in Fig. 4 we plot the case of square lattice with graded fibres and straight-edge quadratic polygons across the fibre/matrix interface, thus introducing a rectification error on such interior boundary. A sub-optimal convergence rate for all three discretizations is expected due to this geometric inconsistency [41] (see also [56] for FEM) and can be clearly observed.

5.2. Adaptive mesh refinement procedure: doubly periodic functionally graded fibre reinforced composite

In order to validate the proposed a-posteriori error estimator we apply the adaptive mesh refinement algorithm (cf. Section 4.1) to the homogenization problem of fibre reinforced doubly periodic composites introduced in the previous section. The analysis focuses on square fibre arrangements for simplicity. We present results corresponding to quadrilateral and Voronoi polygonal discretizations, obtained for order $k = 2, 3$, respectively. Reference solutions are derived resorting to the analytical method proposed in Ref. [55].

In Fig. 5 we report $\#dof-$convergence plots for the cell function components χ_h in the H^1-error norm, for a set of selected fibre grading cases corresponding to isotropic homogeneous fibres with exponential grading and fibre volume fractions $f = 0.4, 0.6$. Efficiency and reliability of the proposed error estimator is clearly observed as the error curves for the adaptive mesh refinement solutions present the optimal slopes $O((\#dofs)^{-k/2})$ for given k and grant significantly lower error levels if compared with homologous (i.e. with the same number $\#dofs$ of degrees of freedom) uniform mesh refinement solutions.

In Fig. 6, for illustrative purposes, we report the cases of a homogeneous (resp. a graded composite) with different volume fractions and

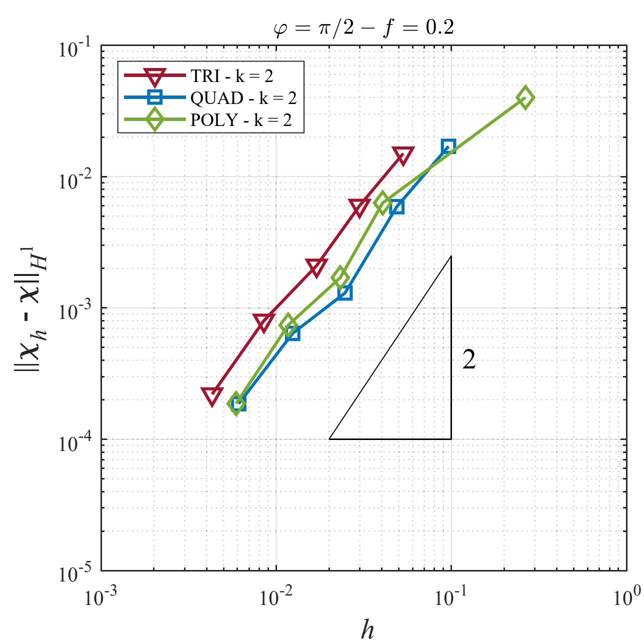

Fig. 4. Doubly periodic composite. Sub-optimal $h-$convergence plots for $k = 2$, for the cell function $\chi(y)$ in the H^1-error norm for uniform mesh refinement and *rectified* fibre/matrix interface. Square lattice, isotropic homogeneous fibres: $\xi = 500$, $\delta = \rightarrow \infty$.

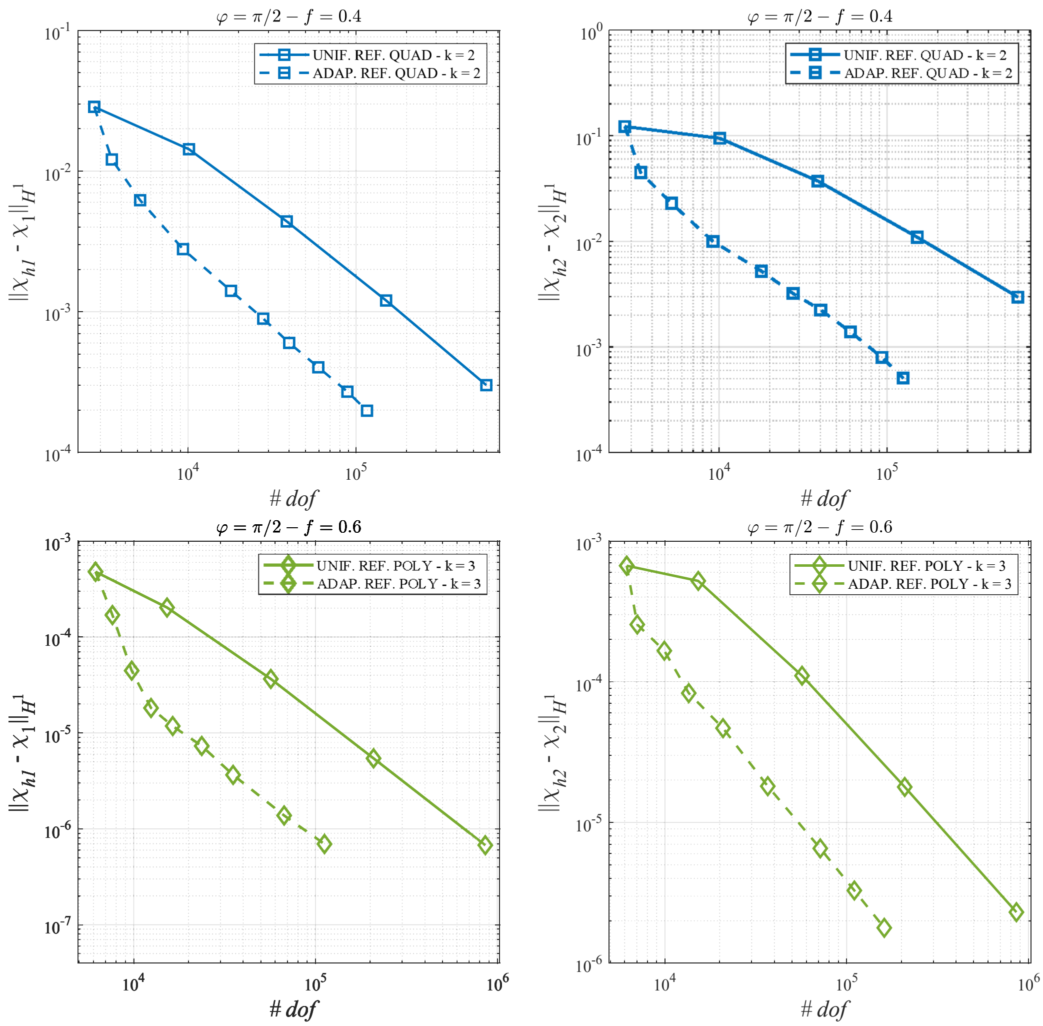

Fig. 5. Doubly periodic composite. *# dof*−convergence plots for $k = 2, 3$, for the cell function components $\chi_s(s = 1, 2)$ in the H^1−error norm for uniform *vs.* adaptive mesh refinement: square lattice, imperfect interfaces with $\delta = 10$. Left column: isotropic homogeneous fibres with $\xi = 500$. Right column: isotropic exponentially graded fibres with $\xi = 500$, $\omega = 8$, $\delta = 10$. Upper row: $f = 0.4$, $k = 2$. Lower row: $f = 0.6$, $k = 3$.

the relative meshes at different adaptive mesh refinement iterations. The refinement process clearly shows localization of the error depending on the unit cell components and, in particular, in the vicinity of the unit cell fibre/matrix interface, and of the exterior boundary edges along the direction of each Cartesian component of the unit cell function, with more error spreading within the fibre domain in the graded case. These are in fact the areas characterized by the steepest gradient for any of the two unknown field components χ_h.

From the above numerical evidence, it can be inferred that for the relevant case of random composites, where a statistical homogenization approach imply solving for possibly large number of RUC random realizations, the above tool may be utilized as a means of tuning a *computationally efficient* mesh for actual solution of the cell problem at a lower computational cost than using a standard uniformly refined mesh. This point is addressed in the following section.

5.3. Statistical homogenization of random composites

The present section is devoted to the application of the proposed and validated adaptive mesh refinement strategy to the crucial issue of numerical estimation of the RUC size for random lattices, assuming statistically homogeneous microstructures, yielding an isotropic effective behaviour.

In this view, a quantitative estimation of the RUC size plays an important role from accuracy and computational efficiency standpoints, since the effective modulus $G^{\#}$, obtained by Eq. (15) is a random variable depending on the specific realization of the RUC D. [1] For homogenization purposes, the RUC size is determined in order to ensure a given relative accuracy ϵ of $G^{\#}$. Based on statistical arguments, in order to avoid use of large RUCs requiring heavy computational effort, use of smaller RUCs might be compensated by averaging over higher numbers of realizations of the microstructure to get a prefixed accuracy [21]. Indeed, recalling that the width of the 95% confidence interval is twice the standard deviation $\sigma_{G^{\#}}$ of $G^{\#}$, i.e. $2\sigma_{G^{\#}}/\mu_{G^{\#}} \le \epsilon$, where $\mu_{G^{\#}}$ denotes the mean value, the standard deviation of $G^{\#}$ resulting from n independent realizations D is given by $\sigma^n_{G^{\#}} = \sigma_{G^{\#}}/\sqrt{n}$, so that n could be chosen according to

$$n \ge 4\,\mathrm{CV}^2_{G^{\#}}/\epsilon^2, \tag{35}$$

where $\mathrm{CV}_{G^{\#}} = \sigma_{G^{\#}}/\mu_{G^{\#}}$ is the coefficient of variation.

The idea is then to solve any of these n realizations, for a given RUC size, using the effective adaptive mesh refinement procedure previously developed and compare with a standard uniform mesh refinement strategy, for the relevant case under consideration where a large number of material domain realizations are needed in order to reach a desired

[1] If the RUC were a representative volume element (RVE), the dispersion of $G^{\#}$ would theoretically vanish.

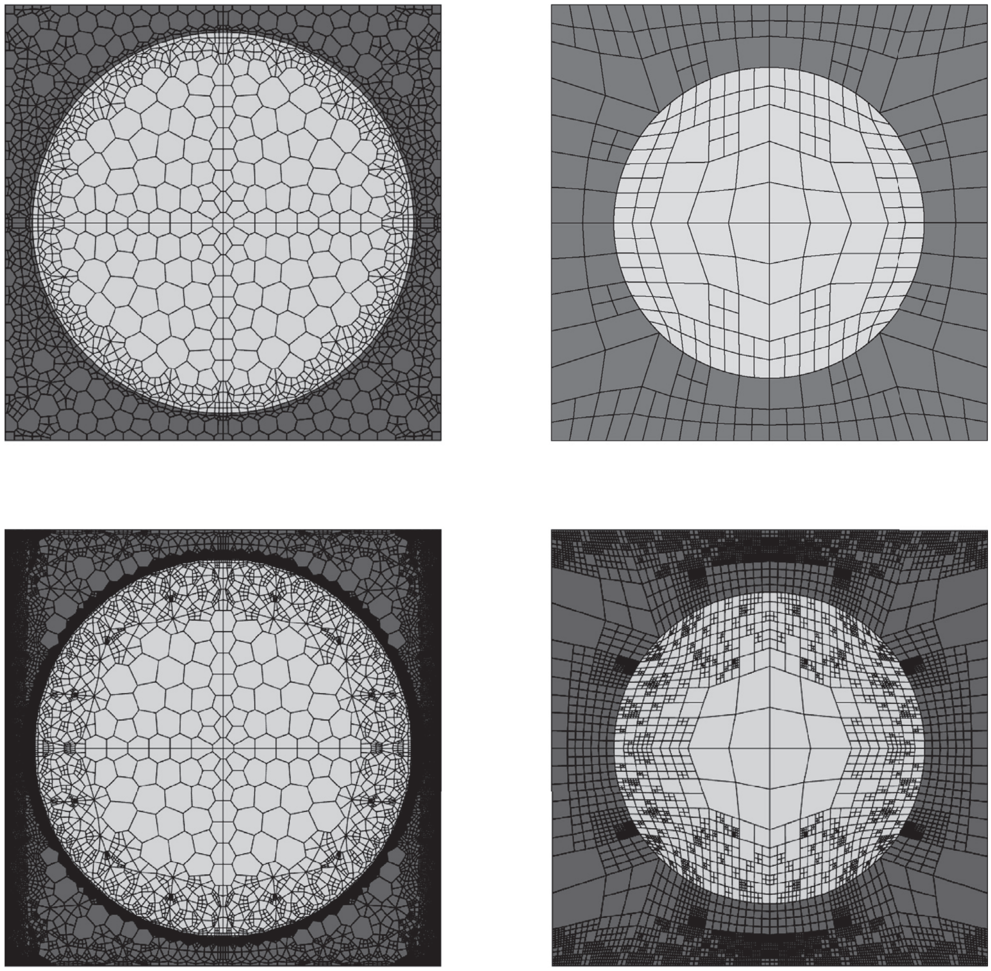

Fig. 6. Adaptive mesh refinement strategy for the cell function components χ_s, $s = 1$-left column, $s = 2$-right column. Square lattice, interfaces with $\delta = 10$. Left column: isotropic homogeneous fibres with $\xi = 500, f = 0.6, k = 2$ with Voronoi discretization. Right column: isotropic exponentially graded fibres with $\xi = 500, \omega = 8, \delta = 10, f = 0.2, k = 3$ with quadrilateral discretization. Upper row: 2− *nd* refinement iteration. Lower row: 6− *th* refinement iteration.

accuracy on the overall material quantities.

To do so, for any given RUC domain realization taken into account in a Monte Carlo simulation (which indeed requires to be meshed and solved), with the aim of comparing computational costs of the two procedures, starting from one initial coarse mesh, we perform a preliminary mesh discretization, adopting, respectively, uniform and adaptive mesh refinements, pursuing a global error level (cf. Eq. (28) and Fig. 5) lower than a prescribed threshold, fixed in 10^{-3} for the current analysis. We then perform Monte Carlo simulations with the two mesh families, comparing accuracy and efficiency of the two approaches. The above statistical homogenization procedure, which follows the line in Ref. [21], is implemented in an in-house numerical toolbox and sketched as follows:

- Set the random composite properties: volume fraction, material parameters of fibres and matrix, grading profile. Set the tolerance for a statistical homogenization procedure convergence, here fixed in 0.5%;
- For each RUC size, determine independent realizations with a number of inclusions with constant radius, according to the pre-set volume fraction and random disposition of fibre centres;
- Initialize meshes by means of the uniform mesh refinement and ACVEM procedure, respectively, for an initial error of 10^{-3};
- For both meshes corresponding to a random realization, solve the homogenization problem and compute the homogenized shear elastic tensor $G^{\#}$
- Repeat until the obtained mean value and variance of the discrete distribution for $G^{\#}$ do not vary any longer up to the preset tolerance.

The two procedures are then compared in terms of the computational cost to reach the statistical homogenization convergence. In the presented numerical simulation, we consider square RUCs with equal, isotropic, exponentially-graded fibres with volume fraction $f = 0.4$, 0.6, stiffness ratio $\xi = 500$, $\omega = 8$, $\delta \to \infty$. The RUC side-to-fibre diameter ratio S ranges from 3.96 to 15.85, meaning that the number of fibres included into a RUC ranges from 8 to 128.

Fig. 7 shows the normalized mean value $\mu_{G^{\#}}/\mathrm{G}^m$ and the dispersion of $G^{\#}$ as a function of the RUC size resulting from $k = 2$, quadrilateral and Voronoi discretizations, obtained with the two meshing strategies. In terms of accuracy, both discretizations seem to converge and it is observed that even a square RUC with $S \geq 8$ (hence, comprising at least 32 fibres) can be used to obtain a fair estimate of $\mu_{G^{\#}}$ in the present case. Table 1 shows the coefficient of variation $\mathrm{CV}_{G^{\#}}$ as a function of the RUC size for the two approaches, together with the ratio between the computational cost of the adaptive mesh refinement (A.M.R.) solution and the uniform mesh refinement (U.M.R.) as a function of RUC size, referring only to the actual computational time of the steps involved in solving the cell problem and computing the effective modulus for the whole realizations examined for a given value S (i.e. without taking into account the computational cost of pre-tuning the mesh).

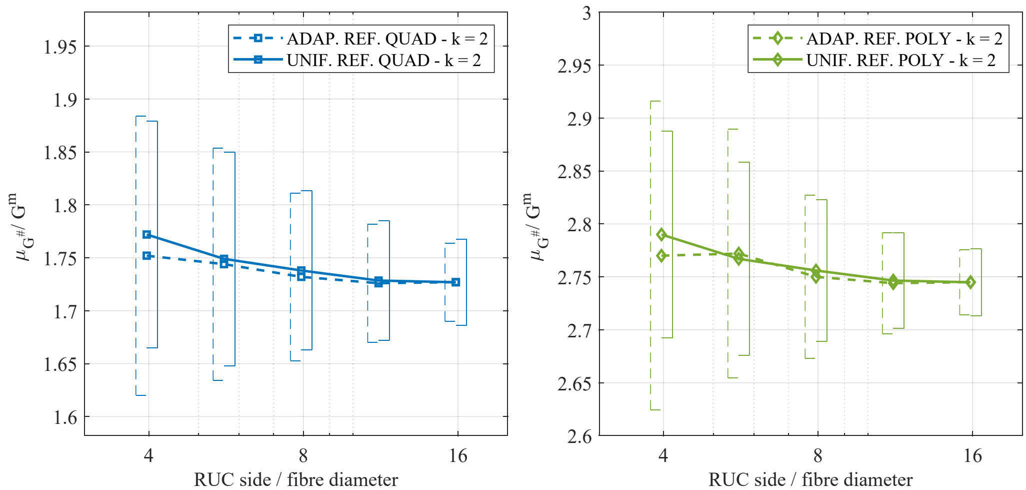

Fig. 7. Statistical homogenization of random composites: determination of RUC size for random graded composites, $f = 0.4$ (quadrilateral - left), $f = 0.6$ (Voronoi - right), for $k = 2$. Normalized mean value $\mu_{G^\#}/G^m$ and dispersion of $G^\#$, comparing adaptive *vs.* uniform mesh refinement strategies as function of the RUC size.

Table 1
Statistical homogenization of random composites: determination of RUC size for random graded composites, $f = 0.4$ (quadrilateral), $f = 0.6$ (Voronoi), for $k = 2$. Coefficient of variation and computational cost ratio of adaptive *vs.* uniform mesh refinement strategies as function of the RUC size.

RUC size	S_1	S_2	S_3	S_4	S_5
	$CV_{G^\#}$ - $f = 0.4$ - Quad				
U.M.R.	0.053	0.050	0.037	0.026	0.015
A.M.R.	0.065	0.055	0.039	0.028	0.018
	comp. cost ratio (A.M.R./U.M.R.)				
	79.4%	75.2%	70.5%	66.8%	61.3%
	$CV_{G^\#}$ - $f = 0.6$ - Poly				
U.M.R.	0.049	0.046	0.033	0.023	0.016
A.M.R.	0.073	0.059	0.039	0.024	0.015
	comp. cost ratio (A.M.R./U.M.R.)				
	88.1%	85.2%	79.5%	72.9%	67.3%

6. Conclusion

In this work we proposed an adaptive curvilinear Virtual Element method of higher order for the asymptotic homogenization of random fibre-reinforced composite materials. The presented approach is based on an a-posteriori error estimator which can drive adaptive mesh refinement of the representative unit cell domain to be studied for a given material setup. Both the curvilinear virtual element technology and the adaptive mesh refinement procedure have been validated on a number of numerical benchmarks taking into account various microstructure configurations. In application to the relevant case of randomly distributed fibres within the composite, following a statistical approach, the aforementioned procedure has been shown to grant accurate and cost-effective homogenized quantities with respect to the standard uniform mesh refinement results.

Conflict of interest and authorship conformation form

- All authors have participated in conception, analysis and interpretation of the data; drafting the article, and approval of the final version.
- This manuscript has not been submitted to, nor is under review at, another journal or other publishing venue.
- The authors have no affiliation with any organization with a direct or indirect financial interest in the subject matter discussed in the manuscript.

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