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A MULTISCALE HOMOGENIZATION SCHEME WITH THE VIRTUAL ELEMENT METHOD

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Abstract. Evaluations and predictions of the behaviour of complex heterogeneous materials such as cementitious mortars, soils, rocks or concretes, require a multi-scale approach. The overall characteristics of these materials strongly depend on processes that are occurring at different length scales. Various scale-levels are required to account for the different mechanisms that control the behaviour at different levels of detail. Among the different multi-scale schemes, those based on homogenization procedures are more commonly used due to their versatility. In this research, a consistent homogenized multiscale approach is proposed for modelling mechanical and transport phenomena. A multiscale model, based in the Virtual Element Method (VEM), is implemented in a VEM^2 setting. VEM allows for a great flexibility in the mesh, and is a powerful tool to characterize the complex RVEs geometries, reducing the amount of elements needed and hence saving time and resources.

1 INTRODUCTION

In the last years great progress has been made in developing constitutive models for composite materials. One area of particular interest has been multiscale formulations, which links the behaviours of different scales and analyses the overall response of heterogeneous material. These approaches generally use relative simple constitutive assumption for the components, and leave aside purely phenomenological assumptions. The behaviour of the lower scale is represented by the so called Representative Volume Element (RVE) or unit cell, which is the smallest volume possible that will provide an accurate representation of the whole domain.

The proposed framework is made for semi-concurrent models. In these models the primary field variables (strain, temperature gradient, etc.) of the coarse-scale are inserted as a Dirichlet boundary condition in the fine-scale. After solving the problem, the dual variables (stress, flux, etc.) and operators (constitutive tensor, thermal conductivity tensor, etc.) are homogenized and used in the coarse-scale. In essence, for each point of the coarse-scale a new fine-scale analysis must be made, which makes the process computationally demanding. Generally this is done using finite element analysis, on a so called 'FE^2' scheme.

A semi-concurrent multiscale model based in the Virtual Element Method (VEM) will be presented in this work. VEM was originated from techniques used in the Mimetic Differences Method, but later introduced as a generalization of the FEM. It use polytopal meshes and allows many interesting possibilities such as allowing hanging nodes, improving adaptivity and mesh flexibility. Though the method is still in its early stages is has been shown to be robust when dealing with highly irregular meshes and complex constitutive behaviours. The mesh flexibility is of particular interest for multiscale analysis, as it allows for simpler meshes with fewer elements, and hence reduces the computational time.

The work is organized as follows: The variational formulations for the mechanical and diffusion problems are stated in Section 2. A thermodynamic background for thermo-plastic materials is described in Section 3, detailing the energetically complementary variables involved in the problem, the derivation of Coleman's equations and the dissipation of each physical process. A semi-concurrent multiscale setting using a thermodynamically consistent framework, is proposed in Section 4. A brief overview of the VEM and the discretization of the problem is presented in Section 5. Some applications and potential developments in Section 6. Finally, some conclusions are compiled in Section 7.

2 FORMULATIONS FOR MECHANICAL AND DIFFUSION PROBLEMS

Mechanical problem The problem is to find displacements $\mathbf{u} : \Omega \to \mathbb{R}^d$, such that

$$\begin{cases} -\boldsymbol{\nabla} \cdot \boldsymbol{\sigma} & = \mathbf{f} \quad \text{in } \Omega \\ \mathbf{u} & = 0 \quad \text{on } \Gamma_D \\ \boldsymbol{\sigma} \cdot \mathbf{n} & = 0 \quad \text{on } \Gamma_N \end{cases} \tag{1}$$

where $\boldsymbol{\sigma}$ is the Cauchy stress, $\mathbf{f}$ the body forces, $\mathbf{n}$ is the outward-pointing normal; and Γ_D and Γ_N are the Dirichlet and Neumann boundaries respectively.

Considering the strain $\boldsymbol{\varepsilon} = \boldsymbol{\nabla}^s \mathbf{u}$, and the constitutive relation $\boldsymbol{\sigma} = \boldsymbol{E} : \boldsymbol{\varepsilon}$ (being $\boldsymbol{E}$ the mechanical material operator), the variational form of the problem is then to find an allowable displacement $\mathbf{u}$ such that

$$a(\mathbf{u}, \mathbf{v}) = \int_\Omega \mathbf{f} \cdot \mathbf{v} \, d\Omega \qquad \text{with} \qquad a(\mathbf{u}, \mathbf{v}) = \int_\Omega \boldsymbol{\varepsilon}(\boldsymbol{u}) : \boldsymbol{E} : \boldsymbol{\varepsilon}(\boldsymbol{v}) \, d\Omega \, . \tag{2}$$

Thermal diffusion problem The problem is to find a temperature $\theta : \Omega \rightarrow \mathbb{R}$, such that

$$\begin{cases} \boldsymbol{\nabla} \cdot \boldsymbol{h} & = \mathrm{f} \quad \text{in } \Omega \\ \theta & = 0 \quad \text{on } \Gamma_D \\ \boldsymbol{h} \cdot \mathbf{n} & = 0 \quad \text{on } \Gamma_N \end{cases} \tag{3}$$

where $\boldsymbol{h}$ is the temperature flux.

Considering Flick's law $\boldsymbol{h} = -\boldsymbol{K}\boldsymbol{\nabla}\theta$ (being $\boldsymbol{K}$ the diffusivity tensor), the variational form of the problem is then to find an allowable temperature θ such that

$$a(\theta, \Theta) = \int_\Omega \mathrm{f}\Theta \, d\Omega \qquad \text{with} \qquad a(\theta, \Theta) = \int_\Omega (\boldsymbol{K}\boldsymbol{\nabla}\theta) \cdot \boldsymbol{\nabla}\Theta \, d\Omega \, . \tag{4}$$

3 THERMODYNAMICS OF DISSIPATIVE MEDIA

The thermodynamic framework for the constitutive equations will be summarized in this section for the particular case of small kinematics and neglectable inertial forces.

First and Second law of thermodynamics

Considering the conservation of mass the first law of thermodynamics can be written as

$$\rho \dot{e} = \boldsymbol{\sigma} : \boldsymbol{\nabla}^s \dot{\boldsymbol{u}} + \rho r - \boldsymbol{\nabla} \cdot \boldsymbol{h} \, , \tag{5}$$

being ρ the density of the solid, e the internal energy density, and r the energy source.

The second law of thermodynamics can be expressed as

$$\dot{S} - Q_\theta \geq 0 \qquad \text{or} \qquad \rho \dot{s} \theta - \rho r + \boldsymbol{\nabla} \cdot \boldsymbol{h} - \frac{\boldsymbol{h} \cdot \boldsymbol{\nabla}\theta}{\theta} \geq 0 \, , \tag{6}$$

with S and Q_θ the entropy and entropy flux respectively; and s the entropy density.

Clausius-Duhem inequality

Combining Eqs. (5) and (6), and introducing Helmholtz's free energy density $\psi = e - s\theta$, the Clausius-Duhem inequality can be deduced>

$$-\rho \dot{\psi} - \rho s \dot{\theta} + \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \frac{\boldsymbol{h} \cdot \boldsymbol{\nabla}\theta}{\theta} \geq 0 \, . \tag{7}$$

Coleman's equations

Coleman's equations can be deduced stating that Eq. (7) must be null for elastic cycles>

$$s = -\frac{\partial \psi}{\partial \theta} \quad , \quad \boldsymbol{\sigma} = \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}^e} \, . \tag{8}$$

Dissipation

By making use of Coleman's equation the dissipation can be expressed as

$$D = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^p - \frac{\boldsymbol{h} \cdot \boldsymbol{\nabla}\theta}{\theta} - \rho \frac{\partial \psi}{\partial \kappa} \dot{\kappa} \geq 0 \, , \tag{9}$$

and decoupled into

$$\text{Intrinsic Dissipation: } D^s = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^p - \rho \frac{\partial \psi}{\partial \kappa} \dot{\kappa} \geq 0 \, , \tag{10}$$

$$\text{Heat transport Dissipation: } D^{th} = -\frac{\boldsymbol{h} \cdot \boldsymbol{\nabla}\theta}{\theta} \geq 0 \, .$$

3.1 Extension to non-local thermodynamics

As can be seen in Nguyen and Andrieux (2005) and Blanco and Giusti (2014), to introduce gradient terms of independent variables the thermodynamic framework needs to be extended. The macroscopic free energy used in this work depends not only on θ but also on $\boldsymbol{\nabla}\theta$, so Helmholtz free energy density must be redefined as

$$\psi = e - s\theta - \boldsymbol{s'} \cdot \boldsymbol{\nabla}\theta \ , \tag{11}$$

with no alteration of the previously defined variables. The vector $\boldsymbol{s'}$, called the entropy vector, can be deduced from analogous Coleman's equations and defined as

$$\boldsymbol{s'} = -\frac{\partial \psi}{\partial \boldsymbol{\nabla}\theta} \ . \tag{12}$$

The dissipations are not modified by this extension.

4 THERMODYNAMICALLY CONSISTENT MULTISCALE SCHEME

In this section, the work done in Rivarola et al. (2017a) and Rivarola et al. (2017b) will be summarized. From this framework the energy balance equations will be derived. It is based on stating the consistency between the Helmholtz's free energy densities and dissipations of the different scales. Additionally, an assumption regarding the primal variables insertion from the coarse-scale to the fine-scale is required. The dual variables and material operators are deduced as a thermodynamic consequence.

Sub-index $(\bullet)_M$ will be used for the properties of the coarse scale, and sub-index $(\bullet)_\mu$ for those of the fine scale. Its important to clarify that the gradient operator is not the same for both scales scales, as it's calculated using different coordinate systems ($\boldsymbol{\nabla}_M \neq \boldsymbol{\nabla}_\mu$). In order to simplify the nomenclature, $\boldsymbol{\nabla}_M(\bullet)_M = [\boldsymbol{\nabla}(\bullet)]_M$ and $\boldsymbol{\nabla}_\mu(\bullet)_\mu = [\boldsymbol{\nabla}(\bullet)]_\mu$.

Axiom 1 - Energy consistency

The energetic consistency is enforced by means of postulating the volume average

$$\psi_M = \frac{1}{V}\int_V \psi_\mu \, dV \ . \tag{13}$$

Assuming that the free energy can be additively decomposed into an elastic free energy and a plastic free energy, so

$$\psi(\boldsymbol{\varepsilon}^e, \theta, \kappa) = \psi^e(\boldsymbol{\varepsilon}^e, \theta) + \psi^p(\kappa) \ . \tag{14}$$

The following expressions for the Helmholtz's free energy densities are adopted

$$\psi^e_\mu = \frac{1}{2}\,\boldsymbol{\varepsilon}^e_\mu : \boldsymbol{E}^e_\mu : \boldsymbol{\varepsilon}^e_\mu \ - \ \frac{1}{2}\frac{\mathscr{C}_\mu}{T_0}\theta^2_\mu \ - \ \theta_\mu \boldsymbol{A}_\mu : \boldsymbol{\varepsilon}^e_\mu \qquad , \qquad \psi^p_\mu = \frac{1}{2}\kappa_\mu H_\mu \kappa_\mu \ , \tag{15}$$

being: $\mathscr{C}$ the volumetric heat capacity; T_0 the reference temperature; $\boldsymbol{A} = \boldsymbol{E} : \boldsymbol{I}\alpha$, with α the thermal dilation coefficient, $\boldsymbol{E}^e$ the elastic constitutive tensor, $\boldsymbol{I}$ the second order identity tensor, H the plastic hardening-softening modulus.

Axiom 2 - Physical primal variables

Displacement and strain homogenization

Without loss of generality the microscale's displacement rate $\dot{\boldsymbol{u}}$ can be decomposed into an average displacement rate, a linear function of the microscale coordinates $\boldsymbol{x}$, and a displacement fluctuation rate:

$$\dot{\boldsymbol{u}}_\mu(\boldsymbol{x}) = \dot{\boldsymbol{u}}_M \; + \; [\boldsymbol{\nabla}\dot{\boldsymbol{u}}]_M \cdot (\boldsymbol{x} - \boldsymbol{x_0}) \; + \; \widetilde{\dot{\boldsymbol{u}}}_\mu \; , \tag{16}$$

being $\boldsymbol{x_0} = \frac{1}{V}\int_V \boldsymbol{x} \, dV$. It is assumed that

$$\dot{\boldsymbol{u}}_M = \frac{1}{V}\int_V \dot{\boldsymbol{u}}_\mu(\boldsymbol{x}) \, dV \; , \quad \text{hence} \quad 0 = \frac{1}{V}\int_V \widetilde{\dot{\boldsymbol{u}}}_\mu \, dV \; . \tag{17}$$

As a consequence

$$[\boldsymbol{\nabla}\dot{\boldsymbol{u}}]_\mu = [\boldsymbol{\nabla}\dot{\boldsymbol{u}}]_M + [\boldsymbol{\nabla}\widetilde{\dot{\boldsymbol{u}}}]_\mu \quad \text{or} \quad \dot{\boldsymbol{\varepsilon}}_\mu = \dot{\boldsymbol{\varepsilon}}_M + \widetilde{\dot{\boldsymbol{\varepsilon}}}_\mu \; , \tag{18}$$

so

$$\dot{\boldsymbol{\varepsilon}}_M = \frac{1}{V}\int_V \dot{\boldsymbol{\varepsilon}}_\mu \, dV \quad \text{and} \quad 0 = \frac{1}{V}\int_V \widetilde{\dot{\boldsymbol{\varepsilon}}}_\mu \, dV \; . \tag{19}$$

It is important to remark that this axiom is postulated for total strains, and is not valid for elastic and plastic strains individually as can be seen in Maugin (1992).

Temperature and temperature gradient homogenization

Proceeding analogously

$$\dot{\theta}_\mu(\boldsymbol{x}) = \dot{\theta}_M \; + \; \left[\boldsymbol{\nabla}\dot{\theta}\right]_M \cdot (\boldsymbol{x} - \boldsymbol{x_0}) \; + \; \widetilde{\dot{\theta}}_\mu \; . \tag{20}$$

Assuming

$$\dot{\theta}_M = \frac{1}{V}\int_V \dot{\theta}_\mu(\boldsymbol{x}) \, dV \; , \quad \text{hence} \quad 0 = \frac{1}{V}\int_V \widetilde{\dot{\theta}}_\mu \, dV \; . \tag{21}$$

Then, as a consequence

$$\left[\boldsymbol{\nabla}\dot{\theta}\right]_\mu = \left[\boldsymbol{\nabla}\dot{\theta}\right]_M + \left[\boldsymbol{\nabla}\widetilde{\dot{\theta}}\right]_\mu \; , \tag{22}$$

and

$$\left[\boldsymbol{\nabla}\dot{\theta}\right]_M = \frac{1}{V}\int_V \left[\boldsymbol{\nabla}\dot{\theta}\right]_\mu \, dV \; . \quad \text{and} \quad 0 = \frac{1}{V}\int_V \left[\boldsymbol{\nabla}\widetilde{\dot{\theta}}\right]_\mu \, dV \; . \tag{23}$$

Corollary 1 - Dual Variables

Macroscopic Stress Tensor: From Eqs. (8) and (13)

$$\boldsymbol{\sigma}_M = \frac{1}{V}\int_V \frac{\partial \psi_\mu}{\partial \boldsymbol{\varepsilon}_M^e} dV = \frac{1}{V}\int_V \left(\boldsymbol{\sigma}_\mu : \frac{\partial \boldsymbol{\varepsilon}_\mu^e}{\partial \boldsymbol{\varepsilon}_M^e} \; - \; s_\mu \frac{\partial \theta_\mu}{\partial \boldsymbol{\varepsilon}_M^e} \; + \; H_\mu \kappa_\mu \frac{\partial \kappa_\mu}{\partial \boldsymbol{\varepsilon}_M^e} \right) dV \; . \tag{24}$$

Macroscopic Entropy: From Eqs. (8) and (13)

$$s_M = \frac{1}{V}\int_V -\frac{\partial \psi_\mu}{\partial \theta_M} dV = -\frac{1}{V}\int_V \left(\boldsymbol{\sigma}_\mu : \frac{\partial \boldsymbol{\varepsilon}_\mu^e}{\partial \theta_M} \; - \; s_\mu \frac{\partial \theta_\mu}{\partial \theta_M} \; + \; H_\mu \kappa_\mu \frac{\partial \kappa_\mu}{\partial \theta_M} \right) dV \; . \tag{25}$$

Macroscopic Entropy vector: From Eqs. (12) and (13)

$$\boldsymbol{s'} = \frac{1}{V}\int_V -\frac{\partial \psi_\mu}{\partial \left[\boldsymbol{\nabla}\theta\right]_M} dV = -\frac{1}{V}\int_V \left(\boldsymbol{\sigma}_\mu : \frac{\partial \boldsymbol{\varepsilon}_\mu^e}{\partial \left[\boldsymbol{\nabla}\theta\right]_M} \; - \; s_\mu \frac{\partial \theta_\mu}{\partial \left[\boldsymbol{\nabla}\theta\right]_M} \; + \; H_\mu \kappa_\mu \frac{\partial \kappa_\mu}{\partial \left[\boldsymbol{\nabla}\theta\right]_M} \right) dV. \tag{26}$$

Corollary 2 - Macroscopic operators

Proposing a macroscopic free energy function analogous to Eq. (15) and the free energy consistency in Eq. (13) homogenization expressions for the operators are deduced.

Macroscopic tangent constitutive tensor

$$\boldsymbol{E}_M = \frac{\partial^2 \psi_M}{\partial \boldsymbol{\varepsilon}_M \partial \boldsymbol{\varepsilon}^e_M} = \frac{\partial \boldsymbol{\sigma}_M}{\partial \boldsymbol{\varepsilon}_M} = \frac{1}{V}\int_V \frac{\partial^2 \psi_\mu}{\partial \boldsymbol{\varepsilon}_M \partial \boldsymbol{\varepsilon}^e_M} dV \,. \tag{27}$$

Macroscopic tensor of thermo-mechanical expansion

$$\boldsymbol{A}_M = -\frac{\partial^2 \psi_M}{\partial \boldsymbol{\varepsilon}^e_M \partial \theta_M} = \frac{\partial s_M}{\partial \boldsymbol{\varepsilon}^e_M} = -\frac{\partial \boldsymbol{\sigma}_M}{\partial \theta_M} = -\frac{1}{V}\int_V \frac{\partial^2 \psi_\mu}{\partial \boldsymbol{\varepsilon}^e_M \partial \theta_M} dV \,. \tag{28}$$

Macroscopic volume heat capacity

$$\frac{\mathscr{C}_M}{T_0} = -\frac{\partial^2 \psi_M}{\partial \theta_M \partial \theta_M} = \frac{\partial s_M}{\partial \theta_M} = -\frac{1}{V}\int_V \frac{\partial^2 \psi_\mu}{\partial \theta_M \partial \theta_M} dV \,. \tag{29}$$

The extension seen in Section 3.1 leads to the existence of additional operators without a counterpart in the coaerse-scale, which are

$$\boldsymbol{A}'_M = -\frac{\partial^2 \psi_M}{\partial \boldsymbol{\varepsilon}^e_M \partial \left[\boldsymbol{\nabla}\theta\right]_M} = \frac{\partial \boldsymbol{s}'_M}{\partial \boldsymbol{\varepsilon}^e_M} = -\frac{\partial \boldsymbol{\sigma}_M}{\partial \left[\boldsymbol{\nabla}\theta\right]_M} = -\frac{1}{V}\int_V \frac{\partial^2 \psi_\mu}{\partial \boldsymbol{\varepsilon}^e_M \partial \left[\boldsymbol{\nabla}\theta\right]_M} dV \,, \tag{30}$$

$$\mathscr{C}'_M = -\frac{\partial^2 \psi_M}{\partial \theta_M \partial \left[\boldsymbol{\nabla}\theta\right]_M} = \frac{\partial \boldsymbol{s}'_M}{\partial \theta_M} = \frac{\partial s_M}{\partial \left[\boldsymbol{\nabla}\theta\right]_M} = -\frac{1}{V}\int_V \frac{\partial^2 \psi_\mu}{\partial \theta_M \partial \left[\boldsymbol{\nabla}\theta\right]_M} dV \,, \tag{31}$$

$$\mathscr{G}'_M = -\frac{\partial^2 \psi_M}{\partial \left[\boldsymbol{\nabla}\theta\right]_M \partial \left[\boldsymbol{\nabla}\theta\right]_M} = \frac{\partial \boldsymbol{s}'_M}{\partial \left[\boldsymbol{\nabla}\theta\right]_M} = -\frac{1}{V}\int_V \frac{\partial^2 \psi_\mu}{\partial \left[\boldsymbol{\nabla}\theta\right]_M \partial \left[\boldsymbol{\nabla}\theta\right]_M} dV \,. \tag{32}$$

Energy Balance - Dissipation consistency

In order to have a fully consistent homogenization procedure, the energy balance is obtained from the dissipation and not from arbitrary potentials. The following expressions of the macroscopic dissipation terms can be obtained for the corresponding homogenization processes

$$D^s_M = \frac{1}{V}\int D^s_\mu \, dV \quad , \quad D^{th}_M = \frac{1}{V}\int D^{th}_\mu \, dV \,. \tag{33}$$

Hence, the energy balance formula for thermal diffusion is

$$\frac{h_M \left[\boldsymbol{\nabla}\theta\right]_M}{\theta_M} = \frac{1}{V}\int \frac{\boldsymbol{h}_{\boldsymbol{\mu}} \cdot \left[\boldsymbol{\nabla}\theta\right]_\mu}{\theta_\mu} \, dV \,. \tag{34}$$

5 THE VIRTUAL ELEMENT METHOD

A summary of the VEM numerical procedure will be given in this section. For more details see da Veiga et al. (2016) and Beirão da Veiga et al. (2014) for the diffusion problem, and Artioli et al. (2017) for the mechanical problem.

5.1 Discretization

Given a domain Ω divided into a mesh τ_h, for a desired order of accuracy k and with the space $\mathbb{P}_k$ of the polynomials of maximum degree k, let us define the local space $V_{k,h}^{El}$ as

$$V_{k,h}^{El} = \left\{ v_h \in \mathrm{H}^1(El) : v_{h|\partial El} \in C^0(\partial El),\ v_{h|e} \in \mathbb{P}_k(e)\ \forall e \subset \partial El,\ \Delta v_h \in \mathbb{P}_{k-2}(El) \right\},$$

where h is a mesh parameter, El is an element of the mesh, ∂El is its border and e an edge. From the definition it can be seen that the base functions in the VEM space are not necessarily explicitly known for the entire domain, they are only known at the boundary of the element.

The global virtual element space is

$$\mathcal{V}_{k,h}^{d} = \left\{ v_h \in \mathrm{H}^1_D(\Omega) \cap C^0(\Omega) : v_{h|El} \in \mathcal{V}_{k,h}^{El}, \forall El \in \mathcal{T}_h \right\} \text{ for the diffusion problem,} \tag{35}$$

$$\boldsymbol{\mathcal{V}}_{k,h}^{m} = \left\{ \boldsymbol{v}_h \in \mathrm{H}^1_D(\Omega) \cap C^0(\Omega) : \boldsymbol{v}_{h|El} \in \boldsymbol{\mathcal{V}}_{k,h}^{El}, \forall El \in \mathcal{T}_h \right\} \text{ for the mechanical problem.} \tag{36}$$

As in FEM the discrete solutions of variational problems are searched:
For the diffusion problem, find $u_h \in \mathcal{V}_{k,h}^d$ such that

$$a_h^d(u_h, v_h) = l_h^d(v_h) \qquad \forall v_h \in \mathcal{V}_{k,h}^d\ . \tag{37}$$

and for the mechanical problem, find $\boldsymbol{u_h} \in \boldsymbol{\mathcal{V}}_{k,h}^m$ such that

$$a_h^m(\boldsymbol{u}_h, \boldsymbol{v}_h) = l_h^m(\boldsymbol{v}_h) \qquad \forall \boldsymbol{v}_h \in \boldsymbol{\mathcal{V}}_{k,h}^m\ . \tag{38}$$

The discrete versions of the bilinear forms are defined element-wise

$$\begin{cases} a_h^d(u_h, v_h) & = \sum_{El \in \mathcal{T}_h} a_h^{d,El}(u_h, v_h) = \sum_{El \in \mathcal{T}_h} \int_{El} (\boldsymbol{K} \nabla u_h) \cdot \nabla v_h \, dEl \\ a_h^m(\boldsymbol{u}_h, \boldsymbol{v}_h) & = \sum_{El \in \mathcal{T}_h} a_h^{m,El}(\boldsymbol{u}_h, \boldsymbol{v}_h) = \sum_{El \in \mathcal{T}_h} \int_{El} \boldsymbol{\varepsilon}(\boldsymbol{u}_h) : \boldsymbol{E} : \boldsymbol{\varepsilon}(\boldsymbol{v}_h) \, dEl \end{cases} \tag{39}$$

As the base functions in the local spaces are not explicitly known inside an element the inclusion of the projector operator is required.

Projection operator For the diffusion problem the local projector operator $\Pi_k^{d,E} : \mathcal{V}_{k,h}^E \to \mathcal{P}_k(E)$ acting on a function $v_h \in \mathcal{V}_{k,h}^E$ yields the polynomial $\Pi_{E,k}(v_h) \in \mathcal{P}_k$ satisfying

$$\underline{a}_h^{d,El}(\Pi_k^{d,El}(v_h), p) = \underline{a}_h^{d,El}(v_h, p) \quad \forall p \in \mathcal{P}_k(El)\ , \tag{40}$$

and for mechanical problems, the local projector operator $\Pi_k^{El} : \boldsymbol{\mathcal{V}}_{k,h}^{El} \to [\mathcal{P}_k(El)]^2$ acting on a function $\boldsymbol{v}_h \in \boldsymbol{\mathcal{V}}_{k,h}^{El}$ is defined by

$$\underline{a}_h^{m,El}(\Pi_k^{m,El}(\boldsymbol{v}_h), \boldsymbol{p}) = \underline{a}_h^{m,El}(\boldsymbol{v}_h, \boldsymbol{p}) \quad \forall \boldsymbol{p} \in [\mathcal{P}_k(El)]^2\ . \tag{41}$$

In this work it is assumed that the coefficients in $\boldsymbol{K}$ and $\boldsymbol{E}$ are constant within each element. Although the base functions are not known in the interior of the elements, the projector can be exactly computed for functions in the local space using from the DOFs using integration by parts. The definitions of the projection operator guarantee exact results when tested against polynomials of degree up to k.

Stiffness matrix The local bilinear form needs to be decomposed into a consistency and a stability term

$$a_h^{d,El}(u_h, v_h) = \underbrace{a_h^{d,El}(\Pi_k^{d,El}(u_h), \Pi_k^{d,El}(v_h))}_{consistency} + \underbrace{\mathcal{S}^{d,El}(u_h - \Pi_k^{d,El}(u_h), v_h - \Pi_k^{d,El}(v_h))}_{stabilization}\,, \tag{42}$$

$$a_h^{m,El}(\boldsymbol{u}_h, \boldsymbol{v}_h) = \underbrace{a_h^{m,El}(\Pi_k^{m,E}(\boldsymbol{u}_h), \Pi_k^{m,El}(\boldsymbol{v}_h))}_{consistency} + \underbrace{\mathcal{S}^{m,El}(\boldsymbol{u}_h - \Pi_k^{m,El}(\boldsymbol{u}_h)), \boldsymbol{v}_h - \Pi_k^{m,El}(\boldsymbol{v}_h))}_{stabilization}\,. \tag{43}$$

The consistency term approximates the bilinear form using the projection operator, while the stabilization term is applied to the high order terms ($> k$) whose contribution is left out by the projector. The later is taken simply as the scalar product of the values at the DOFs of the difference between the VEM function and its projection,

$$\mathcal{S}^{d,El}(u_h - \Pi_k^{d,El}(u_h), v_h - \Pi_k^{d,El}(v_h)) = \boldsymbol{K} \sum_{l=1}^{n_{k,D}^{El}} \text{dof}_{\,l}(u_h - \Pi_k^{d,El}(u_h))\ \text{dof}_{\,l}(v_h - \Pi_k^{d,El}(v_h)), \tag{44}$$

$$\mathcal{S}^{m,El}(\boldsymbol{u}_h - \Pi_k^{m,El}(\boldsymbol{u}_h), \boldsymbol{v}_h - \Pi_k^{m,El}(\boldsymbol{v}_h)) = \tau \sum_{l=1}^{2n_{k,D}^{El}} \text{dof}_{\,l}(\boldsymbol{u}_h - \Pi_k^{m,El}(\boldsymbol{u}_h))\ \text{dof}_{\,l}(\boldsymbol{v}_h - \Pi_k^{m,El}(\boldsymbol{v}_h))\,, \tag{45}$$

where dof_l is the value at the l-th DOF, and τ is a material parameter which for linear elasticity is constant and dependent on Young's modulus and Poisson's ratio.

By defining a base for the local spaces $\{\varphi_i\}_{i=1,\ldots,n_{k,D}^{El}}$ and $\{\boldsymbol{\varphi}_i\}_{i=1,\ldots,2n_{k,D}^{El}}$, where each function takes the value 1 at its associated DOF and 0 otherwise, the stiffness matrix results

$$\left[k^{d,El}\right]_{ij} = a_h^{d,El}(\varphi_i, \varphi_j) \qquad i,j = 1,\ldots,n_{k,D}^{El}\,, \tag{46}$$

$$\left[k^{m,El}\right]_{ij} = a_h^{m,El}(\boldsymbol{\varphi}_i, \boldsymbol{\varphi}_j) \qquad i,j = 1,\ldots,2n_{k,D}^{El}\,. \tag{47}$$

The assembly of the global matrices system is done as in standard FEM.

Loading terms As the base functions are known on the boundaries surface load terms are treated just as in standard FEM. Volumetric terms will not be considered in this work.

6 APPLICATIONS AND POTENTIAL DEVELOPMENTS

Detail simulations of composite materials must take into account the different components along with their different properties. The flexibility of VEM meshes for modelling complex structures integrates well with multiscale analysis, to simply the analysis of the RVEs. For example, in the cases where a component has a much higher rigidity than the surrounding materials being able to use arbitrary polynomials can be capitalized by meshing the rigid element as a single element. Since only a small variation in the variable field will appear in the rigid element the solution will not be compromised.

Having simpler meshes in the fine-scale has further potentially advantages for non-linear problems. Multiscale non-linear analysis require iterative solving on both scales, making the process complicated and computationally demanding. Additionally it requires storing the information of the multiple RVEs solutions. Hence being able to simplify the analysis and reduce the DOFs of the lower scales is incredibly useful, as it saves both computer time and memory.

Another application of the VEM is its capability as a domain decomposition method. Due to the mesh flexibility any part of the domain can be split into several subdomains, each one with its own new mesh, without greatly affecting the system. When part of the mesh is refined only the elements in that subdomain are affected, so there is no need to compute an entirely new stiffness matrix for the problem. This is of particular interest in failure or cracking analysis. Initially a coarse mesh can be used, and refine only the critical sections as the analysis progresses. The same idea can also be applied to interface elements, adding them only around elements with high stress. Hence VEM can be used for cracking analysis without modifying the formulation nor implementation, unlike complex methods like XFEM or XFEM. Integrated into a multiscale scheme this allows for a coarse mesh to be used in the macro-scale, refining it where and when necessary, reducing computational time and without the need of additional programming.

7 CONCLUSIONS

A thermodynamically consistent homogenisation base multiscale scheme was analysed and defined in the framework of dissipative constitutive theories. The framework is based in the Helmholtz free energy and dissipation volume average. The Virtual Element Method was explained, and its advantages explained. More applications are expected to surface in the foreseeable future, especially for complex and multi-physical problems.

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