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# Multiscale computational homogenization methods with a gradient enhanced scheme based on the discontinuous Galerkin formulation

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ABSTRACT

When considering problems of dimensions close to the characteristic length of the material, the size effects can not be neglected and the classical (so-called first-order) multiscale computational homogenization scheme (FMCH) looses accuracy, motivating the use of a second-order multiscale computational homogenization (SMCH) scheme. This second-order scheme uses the classical continuum at the micro-scale while considering a second-order continuum at the macro-scale. Although the theoretical background of the second-order continuum is increasing, the implementation into a finite element code is not straightforward because of the lack of high-order continuity of the shape functions. In this work, we propose a SMCH scheme relying on the discontinuous Galerkin (DG) method at the macro-scale, which simplifies the implementation of the method. Indeed, the DG method is a generalization of weak formulations allowing for inter-element discontinuities either at the $\mathcal{C}^0$ level or at the $\mathcal{C}^1$ level, and it can thus be used to constrain weakly the $\mathcal{C}^1$ continuity at the macro-scale. The $\mathcal{C}^0$ continuity can be either weakly constrained by using the DG method or strongly constrained by using usual $\mathcal{C}^0$ displacement-based finite elements. Therefore, two formulations can be used at the macro-scale: (i) the full-discontinuous Galerkin formulation (FDG) with weak $\mathcal{C}^0$ and $\mathcal{C}^1$ continuity enforcements, and (ii) the enriched discontinuous Galerkin formulation (EDG) with high-order term enrichment into the conventional $\mathcal{C}^0$ finite element framework. The micro-problem is formulated in terms of standard equilibrium and periodic boundary conditions. A parallel implementation in three dimensions for non-linear finite deformation problems is developed, showing that the proposed method can be integrated into conventional finite element codes in a straightforward and efficient way.



## 1. Introduction

Nowadays, the numerical simulation of engineering applications with heterogeneous materials poses many mathematical and computational challenges. In theory, such problems can be directly solved by using a standard finite element procedure. However, it requires the mesh size $h$ to be smaller than the heterogeneities size, i.e. $\epsilon : h < \epsilon$, and if $\epsilon$ is small, the simulation may not be performed due to the enormous number of the degrees of freedom. An effective remedy, which is known as the computational homogenization, has been developed to link up straightforwardly the responses of the large scale problems, also called the macroscopic problems, to the behavior of the smaller scale problems, also called the microscopic problems, where the presence of heterogeneities is considered. The basic ideas of the computational homogenization approach have been presented in papers by Michel et al. [1], Terada et al. [2], Miehe et al. [3,4], Kouznetsova et al. [5–7], Kaczmarczyk et al. [8], Peric et al. [9], Geers et al. [10] and references therein, as a non-exhaustive list. By this technique, two boundary value problems are defined at two separate scales, one is defined at the microscopic scale and one is defined at the macroscopic scale. Such an approach does not require the macroscopic constitutive response to be known a priori and enables the incorporation of both geometrical and material non-linearities [11]. The macroscopic material law is extracted from the analysis of the microscopic boundary value problem (BVP), which is defined by a representative volume element (RVE) with a suitable boundary condition related to the macroscopic quantities. This procedure does not lead to a closed-form of the macroscopic constitutive law, but the stress–strain relation is always available through the resolution of the BVPs.

The classical multiscale computational homogenization approach (so-called the first order multiscale computational homogenization approach – FMCH) provides a versatile tool to model the micro–macro transitions and is based on the standard continuum theory [1–5,9,10]. For a given macroscopic deformation gradient tensor, the stress and the associated material tangent are

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estimated from the response of the micro-structure, see Fig. 1. Similar first order computational homogenization schemes have also been developed for material layers [12]. Although the first-order scheme accounts for the volume fraction and for the microscopic morphology, the influence of the absolute size of the constituents at the micro-scale is not considered. Indeed, according to the local action principle, the separation of scales must be satisfied in order to capture the equivalent homogeneous state by analyzing the microscopic problem. However, this condition is sometimes violated when the macroscopic length scale and the microscopic length scale gets closer. In this case, the classical FMCH procedure would lead to a solution which is not physical because of the violation of the local action principle. Therefore the classical homogenization procedure cannot capture the high gradient at the RVE level and the size effects cannot be captured in the regions of high deformation gradients [6].

To be able to cover the localization and size effect problems at a given resolution scale, many authors have proposed to use generalized continuum formulations (e.g. Cosserat, couple-stress, strain-gradient, non-local, micromorphic formulations), see [13–19] amongst others. In the generalized continuum theory, the length scale is introduced into the material constitutive law and the method is able to capture the size effects. For the multiscale problems, the generalized continuum can potentially be used at both the macroscopic and the microscopic scales. Recent extensions of the FMCH scheme to the second-order continuum, as for the so-called second-order multiscale computational homogenization (SMCH) [6–8], provide a systematic way to couple the strain-gradient continuum at the macro-scale with the classical continuum at the micro-scale, see Fig. 1. In this scheme, both the deformation gradient and its gradient are used at each macroscopic material point to define the microscopic boundary condition. The macroscopic stress and higher-order stress are computed by using the generalized version of the Hill–Mandel macro-homogeneity condition.

To solve the strain-gradient problem at the macro-scale, the addition of the high-order terms in the generalized internal virtual work leads to many complications in the numerical treatment of the finite element framework. With the conventional displacement-based finite element method, this requires not only the continuity of the displacement field but also the continuity of its first derivatives. In other words, at least the $\mathcal{C}^1$ continuity of the interpolation shape functions must be used. When solving the strain-gradient problems, the $\mathcal{C}^1$ finite elements have been successfully developed, see [20,21]. Alternative approaches consider a

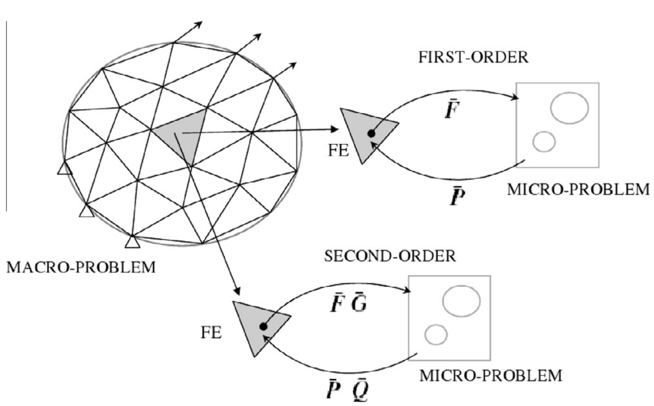


**Fig. 1.** Illustration of first-order and second-order multiscale computational homogenization schemes. The deformation gradient $\bar{\boldsymbol{F}}$ and the first-order stress $\bar{\boldsymbol{P}}$ are used in the first-order scheme while the gradient of deformation gradient $\bar{\boldsymbol{G}} = \bar{\boldsymbol{F}} \otimes \nabla_0$ and the higher-order stress $\bar{\boldsymbol{Q}}$ are added to capture the high-order effects in the second-order scheme.

mixed formulation [22,23] or the micromorphic formulation [19], from which the strain gradient formulation can be recovered. The strategy of introducing another unknown field beside the unknown displacement field in the $\mathcal{C}^1$ element, as in the mixed formulation and in the micromorphic formulation, raises the number of degrees of freedom. Therefore, the use of the $\mathcal{C}^0$ conventional continuous elements is favored. Another effective approach is the continuous–discontinuous Galerkin ($\mathcal{C}^0$/DG) method [24,25]. This approach, which uses $\mathcal{C}^0$ continuous interpolation functions, is formulated in terms of the displacement unknowns only and weakly enforces the continuity of the higher-order derivatives at the inter-element boundaries by using the DG formulation. However, in the mentioned works, only linear elastic materials are considered. In this paper a one-field DG formulation of the strain-gradient theory for finite strains is required.

As a generalization of weak formulations, DG methods allow for the discontinuities of the problem unknowns in the interior of the domain, see [26,27] and their references. The domain is divided into sub-domains on which the integration by parts is applied, leading to boundary integral terms on the subdomain interfaces. The role of these terms is to satisfy the consistency and to enforce weakly the continuity of the problem unknowns. When considering problems involving high-order derivatives, the DG method can also be seen as a way of imposing weakly the high-order continuity. This advantage has been exploited in the mechanics of beams and plates [24,28], of shells [29], and of Mindlin's theory [24,25]. When using DG methods, the discontinuities can be related to the unknown fields and their derivatives or to their derivatives only. The DG methods have also been developed for strain-gradient damage [30] and for gradient plasticity [31,32], in which case the discontinuity of the equivalent strain across inter-element interfaces is weakly enforced. In mathematical analyzes, the DG methods were also used to impose weakly the $\mathcal{C}^0$ continuity of the displacement field [33,34] at the macro-scale when solving, multiscale elliptic problems.

The purpose of this work is to establish a second-order multiscale computational homogenization for finite deformations based on the DG formulation at the macro-scale, while the micro-problem is formulated in terms of standard equilibrium and boundary conditions. The DG method is used to constrain weakly the $\mathcal{C}^1$ continuity by inter-element integrals. The $\mathcal{C}^0$ continuity can be either weakly imposed by the DG formulation or strongly constrained using the conventional $\mathcal{C}^0$ displacement-based finite element. Thus two formulations can be used:

- The full DG formulation (FDG), which constrains weakly the $\mathcal{C}^0$ and $\mathcal{C}^1$ continuities, and
- The enriched DG formulation (EDG) with high-order term enrichments into the conventional $\mathcal{C}^0$ finite element framework.

Considering a DG formulation allows traditional finite element to be considered although the strain-gradient continuum is used. Furthermore, as the shape functions remain continuous with the EDG formulation, the number of degrees of freedom in this case is the same as for conventional $\mathcal{C}^0$ finite elements. On the contrary, the FDG method suffers from an explosion in the number of degrees of freedom as the shape functions are now discontinuous. Nevertheless the FDG formulation is advantageous in case of parallel implementations using face-based ghost elements [35,36]. 3-dimensional implementations of both the EDG and FDG methods are presented in this paper, showing that they can be integrated into conventional parallel finite element codes without significant effort. Non-linear multiscale applications are then presented to demonstrate the efficiency of the method.

The organization of the paper is as follows. In Section 2, the problem statement of the SMCH is recalled. The resolution of the