Proceedings of the 24th UK Conference of the
Association for Computational Mechanics in Engineering
31 March - 01 April 2016, Cardiff University, Cardiff

Guaranteed error bounds for the homogenisation of random materials

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ABSTRACT

The present paper aims to quantify the error due to homogenisation of highly heterogeneous diffusion fields in the solution of linear elliptic PDEs which are common in the modelling of packed particulate composites. This work takes as starting point the pioneering work Oden and Zohdi (1997) and extends it to bound the error in the expectation and second moment of quantities of interest without solving the intractable stochastic fine-scale problem. All the computations involved are deterministic, macroscopic and indepedent of the scale ratio. In the present work, the guaranteed error bounds are re-derived using the Prager-Synge hypercircle theorem. This enabled us to optimise and fully characterise the effectivity of the presented estimates. We also interpret our results in terms of the Reuss and Voigt approaches for the homogenisation of composites. Finally, an efficient procedure is presented to tighten the estimates through the local approximation of the fine-scale model.

Key Words: *error estimation; model error; homogenisation*

1. Overview

Composites play an increasing role in modern mechanical systems. This raises tremendous challenges for computational mechanics. Indeed, the direct modelling of such systems results in intractable problems due to the fast spatial variations of material properties. The analysis of realistic composite systems requires an additional modelling step, whereby the microscopic constituents are substituted by a single material in such a way that this resulting model captures the global behaviour of the system. This process is known as homogenisation (see for example [1, 2]). However, most composite systems used in engineering exhibit a weak scale separation. Worse still, the most interesting features of mechanical problems are located in regions where the scale separation is lost altogether, typically in regions of steep gradients (*e.g.* stress concentration in solid mechanics, localised limit-states such as damage, sharp geometrical irregularities, *etc.*). In such cases, the results provided by homogenised schemes may differ significantly from the results that would be obtained by solving the fine-scale problem directly. In this work, we aim to quantify this discrepancy.

Our work builds on the pioneering work [3]. In that paper, the authors introduced two problems, a fine-scale intractable problem ("true" model); and a homogenised tractable problem (surrogate model). Then, solving only the tractable, surrogate model and using ad hoc a posteriori error estimates, the authors were able to compare the solution of both problems. However, this modelling error bounding technique suffers from certain limitations, the most important of which is the fact that the bounds require the computation of terms involving the fine-scale description of the material properties. In practice, this means that the fine-scale heterogeneities need to be meshed, which becomes quickly intractable as the scale ratio increases. Secondly, the error is not strictly bounded, and a *sufficiently fine* macroscopic mesh needs to be used for the bounding properties to hold in practical applications. Finally, the various parameters that affect the quality of the error bounds, not the least of which is the type of homogenised model that is used to obtain an approximate solution to the fine-scale problem, are difficult to characterise and fully optimise.

In the present paper, we addressed the key limitations of this methods. Our fundamental suggestion is to allow for the position of the heterogeneities to be governed by a random process in the fine-scale problem. In this setting, we aim to estimate (a) the expectation of “energy-norm" and of “goal-oriented" measures of the error (*i.e.* statistical average) and (b) the moments of these measures (*i.e.* statistical dispersion, see fig. 1).

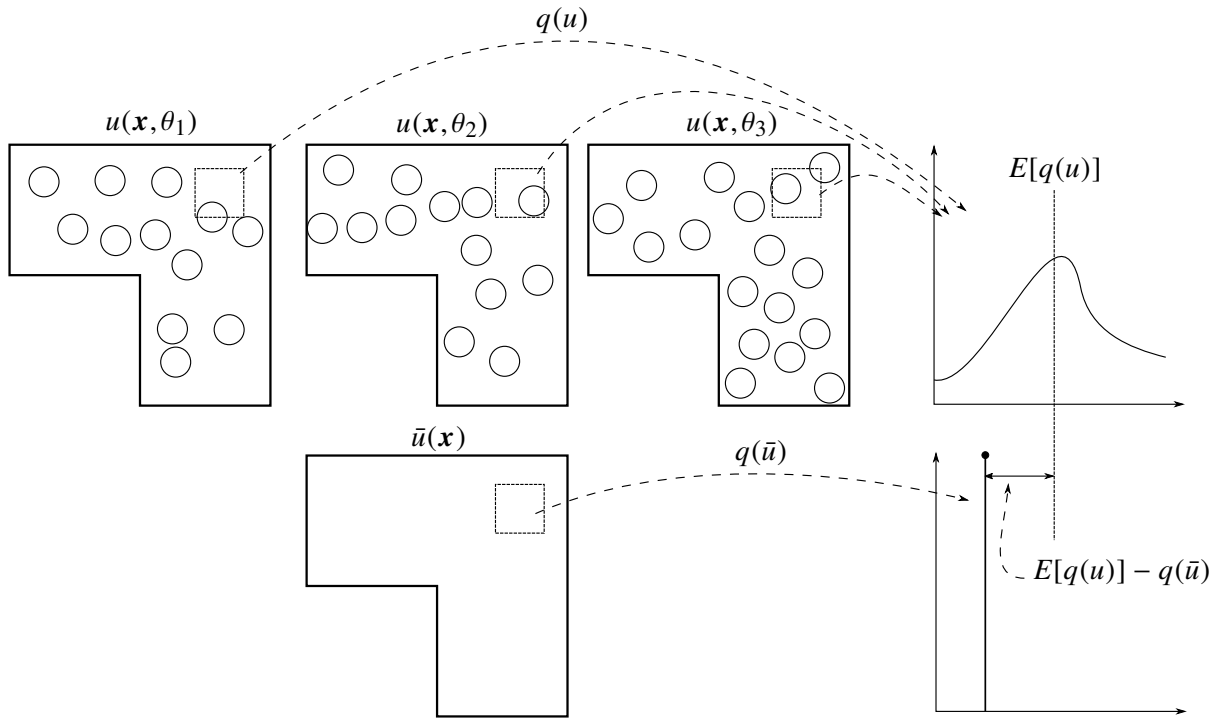

Figure 1: The quantity of interest of the “true model”, $q(u)$, is a probability density function, while it is a scalar in the surrogate model, $q(\bar{u})$. We aim to compare the expectation of both quantities.

In addition to being a realistic modelling setting for heterogeneous media, the direct consequence of this choice is that the computation of the error bounds only involves an integral of a function that, under weakly restrictive assumptions, varies slowly in space. This allows the application of upscaling error bounding without any restriction in terms of scale ratio.

Our second contribution is the development of a general error bounding framework in which the efficiency of the error estimates can be fully characterised and controlled. In order to achieve this difficult task, we propose to base our bounding approach on the Prager-Synge hypercircle theorem[4]. The resulting error bounds are strictly guaranteed and the “true” model is approximated by a pair of surrogates generated from different homogenisation schemes associated with complementary discretisation techniques (namely the compatible and the admissible FEM), instead of single field as proposed in [3]. This pair exhibits very strong similarities to those used to derive the classical Reuss-Voigt bounds for effective medium properties. Such an interesting property will give us a very strong background to characterise, both intuitively and mathematically, and to fully optimise the efficiency of the error estimates (*i.e.* minimise the remaining uncertainty on predicted quantities). One of the possible forms for the error bound is

$$R(\bar{\phi}^h) - \eta\eta_\phi \leq q(u) - q(\bar{u}^h) \leq R(\bar{\phi}^h) + \eta\eta_\phi \tag{1}$$

where R is the residue, $\bar{phi}^h$ is an homogenised approximation to the solution of the dual problem, and η and η_ϕ are upper bounds for the error in energy norm for the primal and dual problem.

Once this new framework has been established, we proceeded as in [5] and show that more accurate and guaranteed estimates can be obtained through locally replacing the homogenised surrogates by the “true”

microscopic model. We call *adaptive modelling* this dynamic, hybrid approximation with elements of the "true" and surrogate model working together towards the accurate bounding of engineering quantities of interest. New local error indicators will also be presented to guide this adaptive modelling process.

2. Numerical example

The methodology is applied to the cylinder head of an engine(fig. 2). At the bottom of the cylinder a temperature of $460K$ is prescribed. At the fins and the upper face it is assumed that a flux of $200W \cdot m^{-2}$ exits the body, while it is assumed that there is no heat exchange in the hole and lateral surfaces. The body is made of matrix enriched with particles. The thermal conductivity of the matrix is $460W/(m \cdot K)$, while the conductivity of the inclusions is $230W/(m \cdot K)$. The inclusions add up to 20% of the volume of the domain. We assume that the probability of being inside an inclusion is the same on every point of the domain and it coincides with the volume fraction. Hence, the expectation of the conductivity $E[k]$, is equal to $vk_p + (1-v)k_m$ and the expectation of its inverse $E[k^{-1}]$ is equal to $v/k_p + (1-v)/k_m$ on every point of the domain. An accurate description of those two functions $E[k]$ and $E[k^{-1}]$ is fundamental for the computation of the error bounds. The quantity of interest is the average temperature on the upper face. The domain was discretised with roughly 1.5 million linear tetrahedrons. The application of the Prager-Synge hypercircle theorem requires two approximate homogenised solutions, namely a kinematically admissible solution (KA) and a statically admissible solution. The KA approximations were obtained using rule of mixture, while the SA approximations were obtained using inverse rule of mixture. The resulting temperature field can be seen in fig. 2 while the bounds can be found in table 1.

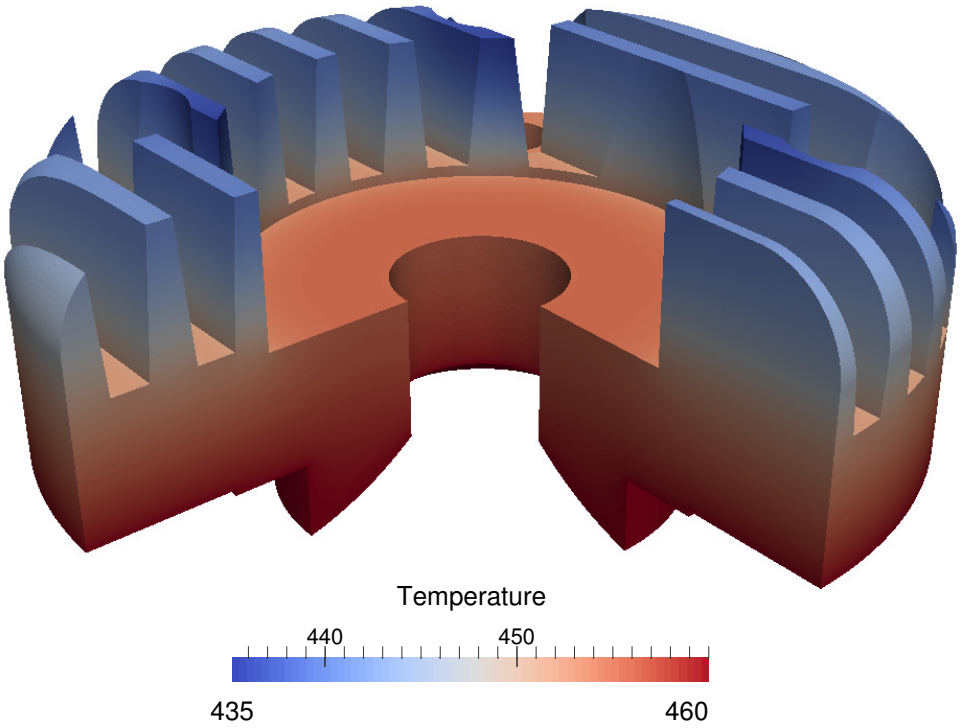

Figure 2: Temperature field of the cylinder head

$q(\bar{u}^h)$	$\zeta_l \leq$	$q(u) - q(\bar{u}^h)$	$\leq \zeta_u$	$\zeta_l + q(\bar{u}^h) \leq$	$q(u)$	$\leq \zeta_u + q(\bar{u}^h)$
445.8	-1.503	Intractable	0.002728	444.3	Intractable	445.8

Table 1: ζ_l and ζ_u represent both lower and upper bounds respectively for $q(u) - q(\bar{u})$, while $\zeta_l + q(\bar{u}^h)$ and $\zeta_u + q(\bar{u}^h)$ are lower and upper bounds for the quantity of interest itself. The direct computation of $q(u)$, the exact quantity of interest, is intractable.

Acknowledgements

The authors would like to acknowledge the financial support of the Framework Programme 7 Initial Training Network Funding under grant number 289361 "Integrating Numerical Simulation and Geometric Design Technology". The authors also acknowledge financial support of EPSRC under grant EP/J01947X/1: "Towards rationalised computational expense for simulating fracture over multiple scales (RationalMSFrac)", and thank Dr Claire Heaney for sharing the code that allowed us to generate realisations of random particulate composites.

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