A posteriori error estimation for POD-based reduced order modelling with application in homogenisation

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Abstract

In this paper, we present an upper bounding technique for reduced order modelling applied to homogenisation. The error estimate relies on the construction of a reduced model for the stress field. Upon ensuring that the reduced stress satisfies the equilibrium in the finite element sense, we can indeed obtain the desired bounding property. We show that the sharpness of the estimate can be seamlessly controlled by changing the parameters of the reduced order model for the stress field.

Keywords: Error estimation; Reduced Order Modelling; Computational Homogenisation; Constitutive Relation Error

1. Introduction

Reduced order modelling is becoming an increasingly popular tool to solve parametrised, stochastic or time-dependent problems (see for instance [1, 2, 3, 4, 5, 6, 7]). However, the field of error estimation for such techniques is not mature yet. In the applied mathematics community, reliable error estimates and error bounding techniques have been developed for the Reduced Basis Method [8], and the Galerkin-POD approach [9], but such methods require a strong background in numerical analysis in order to be understood and implemented. In the engineering community, some empirical methods based on hierarchical enrichment [10] or the Dual-Weighted Residual method [11] have been proposed for the Galerkin-POD, but the resulting estimates do not have bounding properties.

In this contribution, we reconcile these two visions of the problem by proposing an "engineer-friendly" error bounding technique for projection-based reduced order modelling, which we specialise to linear elasticity. The estimate relies on the constitutive relation error, which only requires to manipulate the concepts of displacement and stress admissibilities. The paper is strongly inspired by the work proposed in [12], which applies a similar concept, albeit in a different setting (estimation of the average error introduced by a Proper Generalised Decomposition over the considered parameter space).

Specifically, we apply the Galerkin-POD as a reduced order modelling technique for a parametric problem of elasticity formulated in its primal form ("displacement approach") and discretised by the finite element method. The bounding technique proposes to compute a recovered stress field that is admissible in the finite element sense. To obtain such a field, a snapshot-POD is performed for the finite element stress field, which permits to ensure that the numerical complexity of evaluating the reduced order model and associated error estimate does not depend on the size of the reference finite element problem.

The paper is organised as follows. In the first section, we formulate the parametrised problem of elasticity and introduce the reduced order model. In the second section, we introduce the basics of the proposed error estimate, and give some details about its computation. We conclude the paper with some remarks and potential extensions of the work.

2. Reduced order modelling for Parametric problem of elasticity

We formulate the parametrised problem of an elastic body occupying a bounded domain Ω in a physical space of dimension $d \in \{2, 3\}$. We consider that the input quantities characterising the problem of elasticity are functions of a finite set of n_μ scalar variables that are represented by a vector $\underline{\mu} \in \mathcal{P} \subset \mathbb{R}^{n_\mu}$. Let M be an arbitrary point of domain Ω and let $\underline{x} = x_1\,\underline{e}_1 + \ldots + x_d\,\underline{e}_d + \ldots$ be its coordinates in the reference frame $\mathcal{R} = \left(\underline{O}_{\mathcal{R}}, \underline{e}_1, \underline{e}_2, \underline{e}_3\right)$. We look for a sufficiently regular displacement field $\underline{u}(\underline{\mu}) \in \mathcal{U}(\Omega) = \mathcal{H}^1(\Omega)$ that is continuous and satisfies the Dirichlet boundary conditions $\underline{u} = \underline{w}(\underline{\mu})$ on the part $\partial\Omega^{\text{w}}$ of the domain boundary $\partial\Omega$. Any displacement field that satisfies the conditions of regularity

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and the Dirichlet boundary conditions is said to be kinematically admissible and belongs to space $\mathcal{U}^{\mathrm{Ad}}(\Omega;\underline{\mu}) \subset \mathcal{U}(\Omega)$. We introduce the Cauchy stress tensor field $\underline{\underline{\sigma}}(\underline{\mu})$ which belongs to a space $\mathcal{S}(\Omega)$ of sufficiently regular tensor fields. A density of tractions $\underline{t}(\underline{\mu})$ is applied to the structure on the part $\partial\Omega^{\mathrm{t}} = \partial\Omega\backslash\partial\Omega^{\mathrm{w}}$ of the domain. A density of forces denoted by $\underline{b}(\underline{\mu})$ is applied over Ω. D'Alembert's principle of virtual work expresses the static admissibility, or equilibrium, of an arbitrary stress field that belongs to $\mathcal{S}^{\mathrm{Ad}}(\Omega) \subset \mathcal{S}(\Omega)$ as follows:

$$\forall \underline{\mu} \in \mathcal{P},\ \forall\, \underline{u}^{\star} \in \mathcal{U}^{\mathrm{Ad},0}(\Omega), \quad -\int_{\Omega} \underline{\underline{\sigma}}(\underline{\mu}) : \underline{\underline{\epsilon}}(\underline{u}^{\star})\, d\Omega + \int_{\Omega} \underline{b}(\underline{\mu}) \cdot \underline{u}^{\star}\, d\Omega + \int_{\partial\Omega^{\mathrm{t}}} \underline{t}(\underline{\mu}) \cdot \underline{u}^{\star}\, d\Gamma = 0\,, \tag{1}$$

where the vector space of virtual displacements $\mathcal{U}^{\mathrm{Ad},0}(\Omega)$ associated to $\mathcal{U}^{\mathrm{Ad}}(\Omega;\underline{\mu})$ is such that $\mathcal{U}^{\mathrm{Ad},0}(\Omega) = \{\underline{u} \in \mathcal{U}(\Omega)\ \text{sufficiently regular} \,|\, \underline{u}_{|\partial\Omega^{\mathrm{w}}} = \underline{0}\}$. In the previous equation, $\underline{\underline{\epsilon}}(\underline{u}) = \frac{1}{2}(\nabla \underline{u} + \nabla \underline{u}^T)$ is the displacement gradient. The solution of the problem of elasticity is an admissible pair $(\underline{u}, \underline{\underline{\sigma}}) \in \mathcal{U}^{\mathrm{Ad}}(\Omega;\underline{\mu}) \times \mathcal{S}^{\mathrm{Ad}}(\Omega)$ that verifies the isotropic linear constitutive law $\underline{\underline{\sigma}}(\underline{\mu}) = \underset{\sim}{D}(\underline{\mu}) : \underline{\underline{\epsilon}}\big(\underline{u}(\underline{\mu})\big)$ where $\underset{\sim}{D}(\underline{\mu})$ is the fourth-order Hooke's elasticity tensor. Let us define $\underset{\sim}{C}(\underline{\mu}) \overset{\mathrm{def}}{=} \underset{\sim}{D}(\underline{\mu})^{-1}$.

By substitution of the constitutive law into the principle of virtual work, the parametrised problem of elasticity can be recast in the primal variational form, for any $\underline{\mu} \in \mathcal{P}$,

$$\text{Find } \underline{u}^0(\underline{\mu}) \in \mathcal{U}^{\mathrm{Ad},0}(\Omega) \text{ such that } \forall\, \underline{u}^{\star} \in \mathcal{U}^{\mathrm{Ad},0}(\Omega), \quad a(\underline{u}^0(\underline{\mu}), \underline{u}^{\star}; \underline{\mu}) = l(\underline{u}^{\star}; \underline{\mu}) - a(\underline{u}^{\mathrm{p}}(\underline{\mu}), \underline{u}^{\star}; \underline{\mu})\,, \tag{2}$$

where $\underline{u}^{\mathrm{p}}(\underline{\mu}) \overset{\mathrm{def}}{=} \underline{u}(\underline{\mu}) - \underline{u}^0(\underline{\mu})$ is a particular field of $\mathcal{U}^{\mathrm{Ad}}(\Omega;\underline{\mu})$, and the symmetric bilinear form and the linear form associated with the problem of elasticity are respectively defined, for any fields $\underline{v}$ and $\underline{u}^{\star}$ of $\mathcal{U}(\Omega)$, by

$$a(\underline{v}, \underline{u}^{\star}; \underline{\mu}) = \int_{\Omega} \underline{\underline{\epsilon}}(\underline{u}^{\star}) : \underset{\sim}{D}(\underline{\mu}) : \underline{\underline{\epsilon}}(\underline{v})\, d\Omega\,, \qquad l(\underline{u}^{\star}; \underline{\mu}) = \int_{\Omega} \underline{b}(\underline{\mu}) \cdot \underline{u}^{\star}\, d\Gamma + \int_{\partial\Omega^{\mathrm{t}}} \underline{t}(\underline{\mu}) \cdot \underline{u}^{\star}\, d\Gamma\,. \tag{3}$$

2.1. Discretisation

We approximate the solutions to the parametrised elasticity problem, for any $\underline{\mu} \in \mathcal{P}$, by making use of a classical finite element subspace $\mathcal{U}^{\mathrm{h},0}(\Omega)$ of $\mathcal{U}^{\mathrm{Ad},0}(\Omega)$. The approximation $\underline{u}^{\mathrm{h},0}(\underline{\mu}) \in \mathcal{U}^{\mathrm{h},0}(\Omega)$ of $\underline{u}^0(\underline{\mu})$ is found by solving:

$$\text{Find } \underline{u}^{\mathrm{h},0}(\underline{\mu}) \in \mathcal{U}^{\mathrm{h},0}(\Omega) \text{ such that } \forall\, \underline{u}^{\star} \in \mathcal{U}^{\mathrm{h},0}(\Omega), \quad a(\underline{u}^{\mathrm{h},0}(\underline{\mu}), \underline{u}^{\star}; \underline{\mu}) = l(\underline{u}^{\star}; \underline{\mu}) - a(\underline{u}^{\mathrm{p}}(\underline{\mu}), \underline{u}^{\star}; \underline{\mu})\,, \tag{4}$$

In the following, we assume that the finite element space is sufficiently fine so that any measure of the finite element error $\underline{e}^{\mathrm{h}}(\underline{\mu}) \overset{\mathrm{def}}{=} \underline{u}^{\mathrm{h}}(\underline{\mu}) - \underline{u}(\underline{\mu})$ is small enough for all $\underline{\mu} \in \mathcal{P}$, with $\underline{u}^{\mathrm{h}}(\underline{\mu}) \overset{\mathrm{def}}{=} \underline{u}^{\mathrm{h},0}(\underline{\mu}) + \underline{u}^{\mathrm{p}}(\underline{\mu})$.

2.2. Projection-based reduced order modelling

Let us introduce a basis $(\underline{\phi}_i)_{i\in[\![1,n_\phi]\!]} \in \left(\mathcal{U}^{\mathrm{h},0}(\Omega)\right)^{n_\phi}$ of a representative subspace $\mathcal{U}^{\mathrm{r},0}(\Omega) \subset \mathcal{U}^{\mathrm{h},0}(\Omega)$ in which $\underline{u}^{\mathrm{h},0}(\underline{\mu})$ will be approximated for any $\underline{\mu} \in \mathcal{P}$. This basis is, for instance, obtained by making use of the Snapshot POD. For any $\underline{\mu} \in \mathcal{P}$, we look for an approximation $\underline{u}^{\mathrm{r}}(\underline{\mu})$ of $\underline{u}^{\mathrm{h}}(\underline{\mu})$ to the parametric problem of elasticity in the form

$$\underline{u}^{\mathrm{h}}(\underline{\mu}) \approx \underline{u}^{\mathrm{r}}(\underline{\mu}) \overset{\mathrm{def}}{=} \underline{u}^{\mathrm{r},0}(\underline{\mu}) + \underline{u}^{\mathrm{h,p}}(\underline{\mu}) \quad \text{where} \quad \underline{u}^{\mathrm{r},0}(\underline{\mu}) = \sum_{i=1}^{n_\phi} \underline{\phi}_i\, \alpha_i(\underline{\mu})\,, \tag{5}$$

where, for simplicity, $\underline{u}^{\mathrm{h,p}}(\underline{\mu}) = \underline{u}^{\mathrm{p}}(\underline{\mu})$. The interpolation weights $(\alpha_i)_{i\in[\![1,n_\phi]\!]}$ can be optimally computed by using a Galerkin formulation of the elasticity problem in the reduced space. The reduced order model corresponding to an arbitrary parameter value $\underline{\mu} \in \mathcal{P}$ reads

$$\text{Find } \underline{u}^{\mathrm{r},0}(\underline{\mu}) \in \mathcal{U}^{\mathrm{r},0}(\Omega) \text{ such that } \forall\, \underline{u}^{\star} \in \mathcal{U}^{\mathrm{r},0}(\Omega), \quad a(\underline{u}^{\mathrm{r},0}(\underline{\mu}), \underline{u}^{\star}; \underline{\mu}) = l(\underline{u}^{\star}; \underline{\mu}) - a(\underline{u}^{\mathrm{h,p}}(\underline{\mu}), \underline{u}^{\star}; \underline{\mu})\,. \tag{6}$$

This small system of equations can be solved inexpensively, for any parameter value $\underline{\mu}$ of interest.

3. *A posteriori* error estimation

3.1. Definition of the interpolation error bound

For any $\underline{\mu} \in \mathcal{P}$, the reduced order model delivers a kinematically admissible displacement field $\underline{u}^{\mathrm{r}}(\underline{\mu}) \in \mathcal{U}^{\mathrm{Ad}}(\Omega;\underline{\mu})$. However, the stress field $\underline{\underline{\sigma}}^{\mathrm{r}}(\underline{\mu}) \overset{\mathrm{def}}{=} \underset{\sim}{D}(\underline{\mu}) : \underline{\underline{\epsilon}}\left(\underline{u}^{\mathrm{r}}(\underline{\mu})\right)$ does not satisfy the equilibrium in the finite element sense *a priori*. The idea behind the proposed error estimate law, which relies on the constitutive relation error [13] is to post-process an equilibrated stress field $\widehat{\underline{\underline{\sigma}}}(\underline{\mu}) \in \mathcal{S}(\Omega)$ in the finite element sense, called a "recovered" stress field. This admissibility condition reads:

$$\forall\, \underline{u}^\star \in \mathcal{U}^{\mathrm{h},0}(\Omega), \qquad \int_\Omega \widehat{\underline{\underline{\sigma}}}(\underline{\mu}) : \underline{\underline{\epsilon}}(\underline{u}^\star)\, d\Omega = \int_\Omega \underline{b}(\underline{\mu}) \cdot \underline{u}^\star\, d\Omega + \int_{\partial\Omega^{\mathrm{t}}} \underline{t}(\underline{\mu}) \cdot \underline{u}^\star\, d\Gamma\,. \tag{7}$$

Theorem. The distance ν^{up} between the stress field $\underline{\underline{\sigma}}^{\mathrm{r}}(\underline{\mu}) = \underset{\sim}{D}(\underline{\mu})\, \underline{\underline{\epsilon}}(\underline{u}^{\mathrm{r}}(\underline{\mu}))$ obtained by direct evaluation of the reduced order model and the recovered stress field $\widehat{\underline{\underline{\sigma}}}(\underline{\mu})$ can be used to bound the error of reduced order modelling $\underline{e}^{\mathrm{r}} \overset{\mathrm{def}}{=} \underline{u}^{\mathrm{r}}(\underline{\mu}) - \underline{u}^{\mathrm{h}}(\underline{\mu})$ as follows:

$$\nu^{\mathrm{up}}(\underline{\mu}) = \|\underline{\underline{\sigma}}^{\mathrm{r}}(\underline{\mu}) - \widehat{\underline{\underline{\sigma}}}(\underline{\mu})\|_{\underset{\sim}{C}(\underline{\mu})} \geq \|\underline{e}^{\mathrm{r}}(\underline{\mu})\|_{\underset{\sim}{D}(\underline{\mu})}\,, \tag{8}$$

where $\|\underline{u}^\star\|^2_{\underset{\sim}{D}(\underline{\mu})} = \left(\int_\Omega \underline{\underline{\epsilon}}(\underline{u}^\star) : \underset{\sim}{D}(\underline{\mu}) : \underline{\underline{\epsilon}}(\underline{u}^\star)\, d\Omega\right)^{\frac{1}{2}}$ is the energy semi-norm associated to an arbitrary displacement field $\underline{u}^\star \in \mathcal{U}(\Omega)$, and $\|\underline{\underline{\sigma}}^\star\|^2_{\underset{\sim}{C}(\underline{\mu})} = \left(\int_\Omega \underline{\underline{\sigma}}^\star : \underset{\sim}{C}(\underline{\mu}) : \underline{\underline{\sigma}}^\star\, d\Omega\right)^{\frac{1}{2}}$ is the energy norm associated to an arbitrary stress field $\underline{\underline{\sigma}}^\star \in \mathcal{S}(\Omega)$.

Proof. Let us write the trivial identity

$$\|\underline{\underline{\sigma}}^{\mathrm{r}}(\underline{\mu}) - \widehat{\underline{\underline{\sigma}}}(\underline{\mu})\|^2_{\underset{\sim}{C}(\underline{\mu})} = \left\| \left(\underline{\underline{\sigma}}^{\mathrm{r}}(\underline{\mu}) - \underline{\underline{\sigma}}^{\mathrm{h}}(\underline{\mu})\right) + \left(\underline{\underline{\sigma}}^{\mathrm{h}}(\underline{\mu}) - \widehat{\underline{\underline{\sigma}}}(\underline{\mu})\right) \right\|^2_{\underset{\sim}{C}(\underline{\mu})}\,, \tag{9}$$

where $\underline{\underline{\sigma}}^{\mathrm{h}}(\underline{\mu}) \overset{\mathrm{def}}{=} \underset{\sim}{D}(\underline{\mu}) : \underline{\underline{\epsilon}}\left(\underline{u}^{\mathrm{h}}(\underline{\mu})\right)$ is the reference finite element stress field. Then, by using the constitutive relation for $\underline{\underline{\sigma}}^{\mathrm{h}}(\underline{\mu})$ and $\underline{\underline{\sigma}}^{\mathrm{r}}(\underline{\mu})$ and the definition of the energy norms for displacement and stress fields respectively, equation (9) can be expanded as follows:

$$\|\underline{\underline{\sigma}}^{\mathrm{r}}(\underline{\mu}) - \widehat{\underline{\underline{\sigma}}}(\underline{\mu})\|^2_{\underset{\sim}{C}(\underline{\mu})} = \|\underline{u}^{\mathrm{r}}(\underline{\mu}) - \underline{u}^{\mathrm{h}}(\underline{\mu})\|^2_{\underset{\sim}{D}(\underline{\mu})} + \|\underline{\underline{\sigma}}^{\mathrm{h}}(\underline{\mu}) - \widehat{\underline{\underline{\sigma}}}(\underline{\mu})\|^2_{\underset{\sim}{C}(\underline{\mu})} + 2\int_\Omega \left(\underline{\underline{\sigma}}^{\mathrm{h}}(\underline{\mu}) - \widehat{\underline{\underline{\sigma}}}(\underline{\mu})\right) : \left(\underline{\underline{\epsilon}}\left(\underline{u}^{\mathrm{r}}(\underline{\mu})\right) - \underline{\underline{\epsilon}}\left(\underline{u}^{\mathrm{h}}(\underline{\mu})\right)\right) d\Omega\,. \tag{10}$$

Recall that both the finite element stress field and the recovered stress field are equilibrated in the finite element sense, and that the finite element displacement field and the displacement field obtained by solving the reduced order model belong to $\mathcal{U}^{\mathrm{h},0}(\Omega) + \{\underline{u}^{\mathrm{p}}(\underline{\mu})\}$. We therefore obtain that the last term in (10) vanishes. The proof is concluded by noticing that $\|\underline{\underline{\sigma}}^{\mathrm{h}}(\underline{\mu}) - \widehat{\underline{\underline{\sigma}}}(\underline{\mu})\|^2_{\underset{\sim}{C}(\underline{\mu})}$ is positive. □

3.2. Construction of the recovered stress field: principle

In order to build the recovered stress field, we propose to build a POD-based reduced order model for the finite element stress. We formally split the finite element stress into two parts, as follows

$$\forall\, \underline{\mu} \in \mathcal{P}, \quad \underline{\underline{\sigma}}^{\mathrm{h}}(\underline{\mu}) = \underline{\underline{\sigma}}^{\mathrm{h},0}(\underline{\mu}) + \underline{\underline{\sigma}}^{\mathrm{h,p}}(\underline{\mu})\,. \tag{11}$$

The first part $\underline{\underline{\sigma}}^{\mathrm{h},0}(\underline{\mu})$ satisfies the homogeneous equilibrium conditions associated with the finite element problem:

$$\forall\, \underline{u}^\star \in \mathcal{U}^{\mathrm{h},0}(\Omega), \qquad \int_\Omega \underline{\underline{\sigma}}^{\mathrm{h},0}(\underline{\mu}) : \underline{\underline{\epsilon}}(\underline{u}^\star)\, d\Omega = 0\,. \tag{12}$$

The second term of splitting (11) is a particular stress field that satisfies the equilibrium in the finite element sense:

$$\forall\, \underline{u}^\star \in \mathcal{U}^{\mathrm{h},0}(\Omega), \qquad \int_\Omega \widehat{\underline{\underline{\sigma}}}^{\mathrm{h,p}}(\underline{\mu}) : \underline{\underline{\epsilon}}(\underline{u}^\star)\, d\Omega = \int_\Omega \underline{b}(\underline{\mu}) \cdot \underline{u}^\star\, d\Omega + \int_{\partial\Omega^{\mathrm{t}}} \underline{t}(\underline{\mu}) \cdot \underline{u}^\star\, d\Gamma\,. \tag{13}$$

The first part $\underline{\underline{\sigma}}^{\mathrm{h,p}}(\underline{\mu})$ will be explicitly defined for any $\underline{\mu} \in \mathcal{P}$, while the complementary part $\underline{\underline{\sigma}}^{\mathrm{h},0}(\underline{\mu})$ will be approximated using the snapshot POD:

$$\underline{\underline{\sigma}}^{\mathrm{h}}(\underline{\mu}) \approx \widehat{\underline{\underline{\sigma}}}(\underline{\mu}) \overset{\mathrm{def}}{=} \underline{\underline{\sigma}}^{\mathrm{r},0}(\underline{\mu}) + \underline{\underline{\sigma}}^{\mathrm{h,p}}(\underline{\mu})\,, \tag{14}$$

where the approximate stress $\underline{\underline{\sigma}}^{\mathrm{r},0}(\underline{\mu})$ is such that it satisfies the homogeneous equilibrium equations

$$\forall\, \underline{u}^\star \in \mathcal{U}^{\mathrm{h},0}(\Omega), \qquad \int_\Omega \underline{\underline{\sigma}}^{\mathrm{r},0}(\underline{\mu}) : \underline{\underline{\epsilon}}(\underline{u}^\star)\, d\Omega = 0\,. \tag{15}$$

3.3. Riesz representation of the parametric static load

Let us build the particular equilibrated (in the FE sense) stress field $\underline{\underline{\sigma}}^{\mathrm{h,p}}(\underline{\mu})$. We assume an affine form of the Neumann boundary conditions and body forces, which reads

$$\begin{aligned} &\forall\, \underline{\mu} \in \mathcal{P},\ \forall\, \underline{x} \in \Omega, \qquad \underline{t}(\underline{x}, \underline{\mu}) = \sum_{i=1}^{n_{\mathrm{t}}} \underline{\bar{t}}_i(\underline{x})\, \gamma_i^{\mathrm{t}}(\underline{\mu})\,, \\ &\forall\, \underline{\mu} \in \mathcal{P},\ \forall\, \underline{x} \in \Omega, \qquad \underline{b}(\underline{x}, \underline{\mu}) = \sum_{i=n_{\mathrm{t}}+1}^{n_{\mathrm{t}}+n_{\mathrm{b}}} \underline{\bar{b}}_i(\underline{x})\, \gamma_i^{\mathrm{b}}(\underline{\mu})\,. \end{aligned} \tag{16}$$

We precompute a set of global finite element vectors $(\widetilde{\psi}_i)_{i\in[\![1,\, n_{\mathrm{t}}+n_{\mathrm{b}}]\!]} \in \left(\mathcal{U}^{\mathrm{h},0}(\Omega)\right)^{n_{\mathrm{t}}+n_{\mathrm{b}}}$ corresponding to the summand of the affine form identities. These pre-computations consists in solving the finite element problems:

$$\begin{aligned} &\forall\, i \in [\![1,\, n_{\mathrm{t}}]\!],\ \forall\, \underline{u}^\star \in \mathcal{U}^{\mathrm{h},0}(\Omega), && a(\widetilde{\psi}_i, \underline{u}^\star; \underline{\mu}_0) = \int_{\partial\Omega^{\mathrm{t}}} \underline{\bar{t}}_i \cdot \underline{u}^\star\, d\Gamma\,, \\ &\forall\, i \in [\![n_{\mathrm{t}}+1,\, n_{\mathrm{t}}+n_{\mathrm{b}}]\!],\ \forall\, \underline{u}^\star \in \mathcal{U}^{\mathrm{h},0}(\Omega), && a(\widetilde{\psi}_i, \underline{u}^\star; \underline{\mu}_0) = \int_{\Omega} \underline{\bar{b}}_i \cdot \underline{u}^\star\, d\Omega\,. \end{aligned} \tag{17}$$

The choice of the bilinear form $a(\,.\,,\,.\,;\underline{\mu}_0)$ is arbitrary.

When evaluating the reduced model for a given parameter $\underline{\mu} \in \mathcal{P}$, we can simply estimate the field $\underline{\widetilde{u}}^{\mathrm{h,p}}(\underline{\mu}) \in \mathcal{U}^{\mathrm{h}}(\Omega)$ by using the formula

$$\underline{\widetilde{u}}^{\mathrm{h,p}}(\underline{\mu}) = \sum_{i=1}^{n_{\mathrm{t}}} \widetilde{\psi}_i\, \gamma_i^{\mathrm{t}}(\underline{\mu}) + \sum_{i=n_{\mathrm{t}}+1}^{n_{\mathrm{t}}+n_{\mathrm{b}}} \widetilde{\psi}_i\, \gamma_i^{\mathrm{b}}(\underline{\mu})\,. \tag{18}$$

It is then easy to verify that the stress field $\underline{\underline{\sigma}}^{\mathrm{h,p}}(\underline{\mu}) \overset{\mathrm{def}}{=} \underset{\sim}{D}(\underline{\mu}_0) : \underline{\underline{\epsilon}}(\underline{\widetilde{u}}^{\mathrm{h,p}}(\underline{\mu}))$ is statically admissible in the finite element sense. Therefore, the quantity $\|\underline{\underline{\sigma}}^{\mathrm{h,p}}(\underline{\mu}) - \underline{\underline{\sigma}}^{\mathrm{r}}(\underline{\mu})\|_{\underset{\sim}{C}(\underline{\mu})}$ is an upper bound for the error measure $\|\underline{u}^{\mathrm{r}}(\underline{\mu}) - \underline{u}^{\mathrm{h}}(\underline{\mu})\|_{\underset{\sim}{D}(\underline{\mu})}$, which will be sharpened in the next paragraph by computing the complement $\underline{\underline{\sigma}}^{\mathrm{r},0}(\underline{\mu})$.

3.4. Snapshot POD for the finite element stress

We apply a snapshot POD technique, and precompute the snapshot set $\{\underline{\underline{\sigma}}^{\mathrm{r}}(\underline{\mu})\,|\,\underline{\mu} \in \tilde{\mathcal{P}}\}$, where $\tilde{\mathcal{P}}$ is a discrete subset of $\mathcal{P}$. By substracting the corresponding values of the previously computed admissible stress component $\underline{\underline{\sigma}}^{\mathrm{h,p}}(\underline{\mu})$, we obtain a set of stress fields $\{\underline{\underline{\sigma}}^{\mathrm{h},0}(\underline{\mu})\,|\,\underline{\mu} \in \tilde{\mathcal{P}}\}$ satisfying the homogeneous equilibrium equations. Now, we compute a singular value decomposition of this set. We look for a set of $\tilde{n}_\phi$ basis tensor fields $(\underline{\underline{\widetilde{\phi}}}_i)_{i\in[\![1,\tilde{n}_\phi]\!]} \in (\mathcal{S}(\Omega))^{\tilde{n}_\phi}$ that are orthogonal with respect to the inner product $<\,.\,,.\,>_{\underset{\sim}{C}(\underline{\mu}_0)} = \int_\Omega .\, : \underset{\sim}{C}(\underline{\mu}_0) : .\, d\Omega$ of space $\mathcal{S}(\Omega)$, and that are solutions to the following optimisation problem:

$$\begin{aligned} &(\underline{\underline{\widetilde{\phi}}}_i)_{i\in[\![1,\tilde{n}_\phi]\!]} = \underset{(\underline{\underline{\phi}}^\star_i)_{i\in[\![1,\tilde{n}_\phi]\!]} \in (\mathcal{S}(\Omega))^{\tilde{n}_\phi},\ <\underline{\underline{\widetilde{\phi}}}^\star_i, \underline{\underline{\widetilde{\phi}}}^\star_j>_{\underset{\sim}{C}(\underline{\mu}_0)} = \delta_{ij}\ \forall (i,j)\in[\![1,\tilde{n}_\phi]\!]^2}{\operatorname{argmin}} \widetilde{J}\left((\underline{\underline{\phi}}^\star_i)_{i\in[\![1,\tilde{n}_\phi]\!]}\right), \\ &\text{where} \quad \widetilde{J}\left((\underline{\underline{\widetilde{\phi}}}^\star_i)_{i\in[\![1,\tilde{n}_\phi]\!]}\right) = \sum_{\underline{\mu}\in\tilde{\mathcal{P}}} \left\| \underline{\underline{\sigma}}^{\mathrm{h},0}(\underline{\mu}) - \sum_{i=1}^{\tilde{n}_\phi} \left\langle \underline{\underline{\sigma}}^{\mathrm{h},0}(\underline{\mu}), \underline{\underline{\widetilde{\phi}}}^\star_i \right\rangle_{\underset{\sim}{C}(\underline{\mu}_0)} \underline{\underline{\widetilde{\phi}}}^\star_i \right\|_{\underset{\sim}{C}(\underline{\mu}_0)}\,. \end{aligned} \tag{19}$$

The solution to optimisation problem (19) can be obtained by solving the eigenvalue problem

$$\underline{\underline{\widetilde{\mathbf{H}}}}^{\mathrm{s}}\, \underline{\widetilde{\gamma}} = \widetilde{\lambda}\, \underline{\widetilde{\gamma}} \quad \text{where} \quad \widetilde{\mathbf{H}}^{\mathrm{s}}_{ij} = \left\langle \underline{\underline{\sigma}}^{\mathrm{h},0}(\underline{\mu}^{\mathrm{s}}_i), \underline{\underline{\sigma}}^{\mathrm{h},0}(\underline{\mu}^{\mathrm{s}}_j) \right\rangle_{\underset{\sim}{C}(\underline{\mu}_0)} \quad \forall\, (i,j) \in [\![1, \tilde{n}_\phi]\!]^2\,. \tag{20}$$

After arranging the eigenvalues $(\widetilde{\lambda}_i)_{i\in[\![1,n_{\mathrm{s}}]\!]}$ of $\underline{\underline{\widetilde{\mathbf{H}}}}^{\mathrm{s}}$ in descending order and denoting the corresponding eigenvectors by $(\underline{\widetilde{\gamma}}_i)_{i\in[\![1,n_{\mathrm{s}}]\!]}$, the solution to the Snapshot POD optimisation problem (19) is given by

$$\forall\, i \in [\![1, \tilde{n}_\phi]\!], \quad \underline{\underline{\widetilde{\phi}}}_i = \sum_{j=1}^{n_{\mathrm{s}}} \underline{\underline{\sigma}}^{\mathrm{h},0}(\underline{\mu}^{\mathrm{s}}_j)\, \frac{\widetilde{\gamma}_{i,j}}{\sqrt{\widetilde{\lambda}_i}}\,. \tag{21}$$

The recovered stress field can now be expressed over the whole parameter domain by the following surrogate model:

$$\forall\, \underline{\mu} \in \mathcal{P}, \quad \underline{\underline{\widetilde{\sigma}}}(\underline{\mu}) = \underline{\underline{\sigma}}^{\mathrm{r},0}(\underline{\mu}) + \underline{\underline{\sigma}}^{\mathrm{h,p}}(\underline{\mu}) = \sum_{i=1}^{\tilde{n}_\phi} \underline{\underline{\widetilde{\phi}}}_i\, \widetilde{\alpha}_i(\underline{\mu}) + \underline{\underline{\sigma}}^{\mathrm{h,p}}(\underline{\mu}) \tag{22}$$

where $(\widetilde{\alpha}_i)_{i\in[\![1,\tilde{n}_\phi]\!]} \in \mathbb{R}^{\tilde{n}_\phi}$ are interpolation coefficients, and are the only unknowns left to be computed when evaluating the reduced model. The next paragraph aims at explaining how to compute these coefficients in an optimal manner.

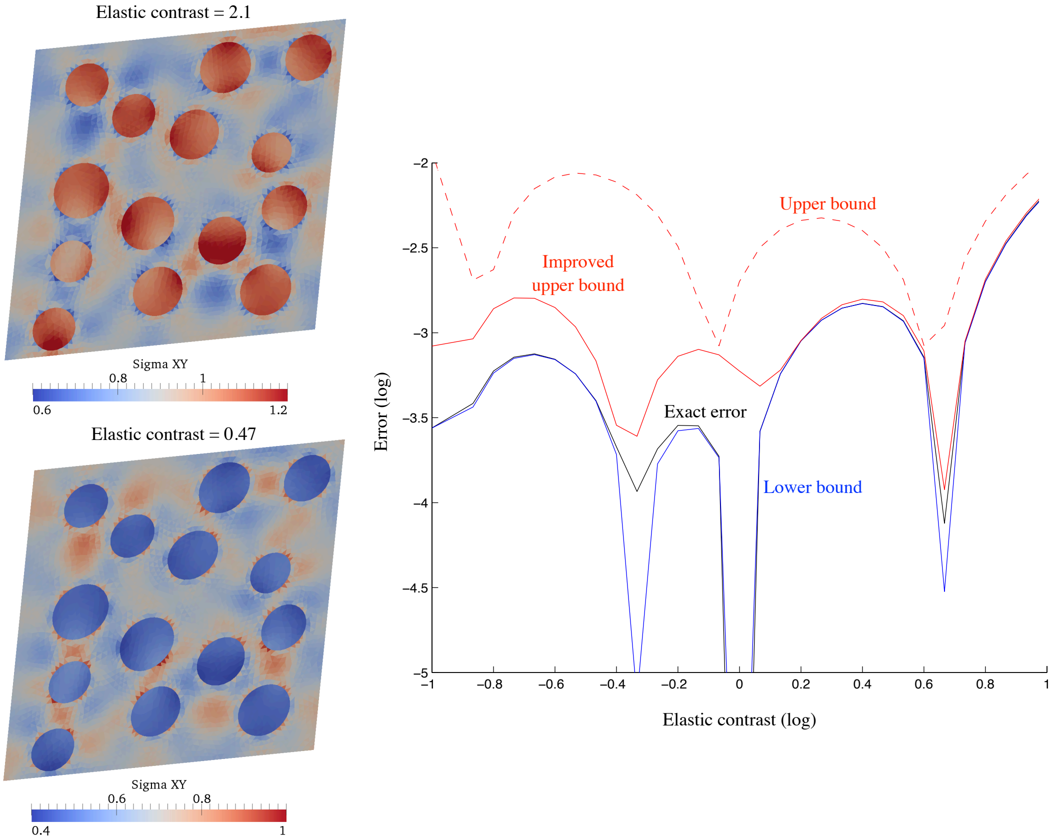

Figure 1: Error estimatation of a POD-based reduced order model in the homogenisation of a particulate composite material.

3.5. *Optimimum upper bound*

When evaluating the reduced order model for a particular $\underline{\mu} \in \mathcal{P}$, the recovered stress $\underline{\underline{\widehat{\sigma}}}(\underline{\mu})$ can be computed optimally in the sense of the maximisation of the efficiency of the error estimate $\nu^{\mathrm{up}}(\underline{\mu})$. In other words, we look for a recovered stress field that is compatible with the surrogate model and is solution to the optimisation problem:

$$\underline{\underline{\widehat{\sigma}}}(\underline{\mu}) = \operatorname*{argmin}_{\underline{\underline{\sigma}}^{\star}(\underline{\mu}) \in \mathcal{S}^{\mathrm{r}}(\Omega;\underline{\mu})} \|\underline{\underline{\sigma}}^{\star}(\underline{\mu}) - \underline{\underline{\sigma}}^{\mathrm{h}}(\underline{\mu})\|_{\underset{\sim}{C}(\underline{\mu})}\,, \tag{23}$$

where the space of admissibility for the reduced stress field is defined by $\mathcal{S}^{\mathrm{r}}(\Omega;\underline{\mu}) = \{\underline{\underline{\sigma}}^{\star} \in \mathcal{S}(\Omega)\,|\,\underline{\underline{\sigma}}^{\star} = \sum_{i=1}^{\tilde{n}_\phi} \underline{\underline{\widetilde{\phi}}}_i\, \alpha_i^{\star} + \underline{\underline{\sigma}}^{\mathrm{h,p}}(\underline{\mu}),\ \forall\,(\alpha_i^{\star})_{i\in[\![1,\tilde{n}_\phi]\!]} \in \mathbb{R}^{\tilde{n}_\phi}\}$. This problem of optimisation can be recast in the variational form

$$\text{Find } \underline{\underline{\widehat{\sigma}}}(\underline{\mu}) \in \mathcal{S}^{\mathrm{r}}(\Omega;\underline{\mu}) \text{ such that } \forall\,\underline{\underline{\sigma}}^{\star} \in \mathcal{S}^{\mathrm{r},0}(\Omega), \quad \int_\Omega \underline{\underline{\widehat{\sigma}}}(\underline{\mu}) : \underset{\sim}{C}(\underline{\mu}) : \underline{\underline{\sigma}}^{\star}\, d\Omega = \int_\Omega \underline{\underline{\epsilon}}\left(\underline{u}^{\mathrm{h}}(\underline{\mu})\right) : \underline{\underline{\sigma}}^{\star}\, d\Omega\,, \tag{24}$$

where the constitutive relation has been used to obtain the right-hand side of the equation, and the space $\mathcal{S}^{\mathrm{r},0}(\Omega)$ is defined by $\mathcal{S}^{\mathrm{r},0}(\Omega) = \{\underline{\underline{\sigma}}^{\star} \in \mathcal{S}(\Omega)\,|\,\underline{\underline{\sigma}}^{\star} = \sum_{i=1}^{\tilde{n}_\phi} \underline{\underline{\widetilde{\phi}}}_i\, \alpha_i^{\star},\ \forall\,(\alpha_i^{\star})_{i\in[\![1,\tilde{n}_\phi]\!]} \in \mathbb{R}^{\tilde{n}_\phi}\}$.

Now, by writing that $\underline{u}^{\mathrm{h}}(\underline{\mu}) = \underline{u}^{\mathrm{h},0}(\underline{\mu}) + \underline{u}^{\mathrm{h,p}}(\underline{\mu})$ and taking into account (15), we obtain the following variational form for the determination of the recovered stress field:

$$\forall\,\underline{\underline{\sigma}}^{\star} \in \mathcal{S}^{\mathrm{r},0}(\Omega), \quad \int_\Omega \underline{\underline{\sigma}}^{\mathrm{r},0}(\underline{\mu}) : \underset{\sim}{C}(\underline{\mu}) : \underline{\underline{\sigma}}^{\star}\, d\Omega = \int_\Omega \underline{\underline{\epsilon}}\left(\underline{u}^{\mathrm{h,p}}(\underline{\mu})\right) : \underline{\underline{\sigma}}^{\star}\, d\Omega\,. \tag{25}$$

4. Application to computational homogenisation

Figure 1 shows numerical results corresponding to the application of the previously described methodology in computational homogenisation. The structure consists of a matrix phase and circular inclusions. The ratio between the young's modulus of the inclusions and the Young's modulus of the matrix, called elastic contrast, is the only scalar parameter of the problem, and ranges from 0.1 to 10. Parameter-independent Dirichlet boundary conditions are applied on the boundary of the domain, as illustrated in the figure.

The snapshot for both the reduced model and the error estimate is computed by sampling the parameter domain at 6 points spaced regularly. The singular value decomposition for the displacement field is truncated at order 3, while the singular value decomposition for the stress field is first truncated at order 3 (curve labelled ”Upper bound”) then at order 4 (curve labelled ”Improved upper bound”). The curves show the two corresponding error estimates, the exact error, which is of course not available in practice, and a lower bound obtained by enriching the reduced model (the SVD for the displacements is truncated at order 4), as a function of the elastic contrast.

When the distance between the upper and lower bound is too large, both bounds can be sharpened by increasing the order of truncation of the corresponding SVDs. If this is insufficient, an enrichment of the snapshot is necessary.

5. Conclusions

We have presented a simple methodology to bound the error introduced when using projection-based reduced order models to solve parametrised elliptic problems. The upper bound can be sharpened by allowing to allocate more computational power to the computation of the bound.

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