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Two-scale Reduced Basis Homogenization under Large Deformations

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Micro Abstract
In this work, the first aim is to solve the task of two-scale homogenization of nonlinear materials for large deformations. We propose a model with a reduced basis for the deformation gradient. The accuracy of the predictions is evaluated online. The main benefit of this approach is the reduction of both CPU time and memory requirements. It also opens opportunities for generalization and further acceleration which are also discussed, e.g. data-driven techniques.

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Introduction

In mechanics of microstructured solids, the question of how to determine or at least approximate homogenized properties under the assumption of scale-separation has been addressed for decades. We focus on strain-driven hyperelasticity for the moment as it can serve as a first step towards more general materials. Hyperelasticity for the geometrically linear description has been intensely investigated by (among others) the authors already [2] and is now adapted to the geometrically nonlinear case.

Previous works on this type of problem include the computational "material map" [3], where the coefficients of a proposed macroscopic constitutive law are linearly interpolated between reference points. Another approach called "R3M" [4] reduces the number of degrees of freedom on the micro-scale by projecting the displacements onto a small-dimensional subspace. In [5], a database of Cauchy-Green tensors and their corresponding free energy function values is constructed using a tensor product approximation of univariate component functions. All of these publications have in common that their numerical sections assume a (quasi) 2D setting. An approach to tackle 3D microstructures was recently published in [1], where neural networks and an approximation of the (inverse) Isomap are combined to yield approximations to the local deformation gradient. The quantities of interest – namely the effective stress and the effective stiffness – then have to be determined outside the reduced order model (ROM).

The key feature of the method proposed here is a ROM with a reduced basis (RB) for the deformation gradient. The basis coefficients are the remaining degrees of freedom. Their computation also provides quantities that are reused for the calculation of the effective response. The second main contribution is an investigation of a sophisticated sampling strategy. It is expected to significantly reduce the amount of pre-computations necessary during the offline phase whilst preserving the accuracy of the ROM. As an additional feature we propose a straightforward way to evaluate (not just approximate) a posteriori the error introduced by the reduced basis model.

1 Notation, problem statement

Let Ω_0 and Ω denote the initial and the current configuration of the solid under investigation, respectively. Positions describing material points are labeled $\mathbf{X}$, those with respect to the current state are marked $\mathbf{x}(\mathbf{X}, t)$. Further kinematic quantities are the deformation gradient $\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}$ and its determinant $J = \det(\mathbf{F})$. We make use of Flory's multiplicative decomposition $\tilde{\mathbf{F}} = J^{-1/3}\mathbf{F}$. Many physical observations suggest an additive split of the hyperelastic energy (density) function $W(\mathbf{F}) = U(J) + \psi(\tilde{\mathbf{F}})$ allowing for independent modeling of the dilatational (U) and the deviatoric (ψ) material properties. The material response to a prescribed deformation gradient will be described in terms of the first Piola-Kirchhoff stress tensor $\mathbf{P}(\mathbf{F}) = \frac{\partial W(\mathbf{F})}{\partial \mathbf{F}}$ and its corresponding fourth-order stiffness tensor $\mathbb{C}(\mathbf{F}) = \frac{\partial^2 W(\mathbf{F})}{\partial \mathbf{F} \partial \mathbf{F}}$. We assume to know these relationships on the micro- but not on the macro-scale. Discrete descriptions of fourth- and second order tensors will be marked by double (matrix) and single (vector) underlined letters respectively, e.g. $\mathbb{C} \leftrightarrow \underline{\underline{C}}$, $\mathbf{P} \leftrightarrow \underline{P}$, ... The transition from microscopic ($\bullet$) to macroscopic ($\bar{\bullet}$) additive quantities is performed through the volume-averaging operator $\bar{\bullet} = \langle \bullet \rangle = \int_{\Omega_0} \bullet \, \mathrm{d}V$. Equilibrium of linear momentum on both scaled is coupled through

$$\begin{aligned} \mathrm{Div}_{\bar{\mathrm{X}}}\left(\bar{\mathbf{P}}\right) + \bar{\mathbf{b}} = \mathbf{0} \qquad & + \text{ macroscopic bc} \\ \mathrm{Div}_{\mathrm{X}}\left(\mathbf{P}\right) = \mathbf{0} \qquad & \langle \mathbf{F} \rangle = \bar{\mathbf{F}} \end{aligned} \tag{1}$$

with the volumetric forces $\bar{\mathbf{b}}$ and, on the micro-scale, periodic fluctuation boundary conditions.

2 Reduced Order Model

The ROM is set up in several steps: first, the RB needs to be introduced, then its coefficients depending on $\bar{\mathbf{F}}$ need to be determined (section 2.1). The effective material response $(\bar{\mathbf{P}}, \bar{\mathbb{C}})$ has to be computed as output (section 2.2). To gain confidence in the model, we propose an online error evaluation (section 2.3). We close this section by some notes on computational issues (section 2.4).

2.1 Reduced basis and its coefficients

We introduce an additive split of the local deformation gradient as

$$\mathbf{F}(\mathbf{x}, t) = \bar{\mathbf{F}}(t) + \underbrace{\mathcal{L}(\mathbf{x})\xi(t)}_{\text{fluctuation}} \qquad \langle \mathcal{L} \rangle = \mathbf{0} \tag{2}$$

where the fluctuations are the application of a temporally constant, linear, zero-average localization operator $\mathcal{L}$ to the spatially constant ("global") coefficients ξ. The space of all kinematically admissible fluctuations is spanned by $\mathcal{L}$, thus any ξ satisfies the microscopic boundary conditions, cf. (1). The operator $\mathcal{L}$ will be determined offline (section 3), thus, in order to evaluate the local material law for a prescribed $\bar{\mathbf{F}}$, only ξ is unknown.

The next ingredient is an effective potential

$$\bar{\Pi} = \bar{W} - W_{\text{ext}} \;\rightarrow \min_{\langle \mathbf{F} \rangle = \bar{\mathbf{F}}} ! \tag{3}$$

which we seek to minimize with respect to all admissible $\mathbf{F}$. This is physically motivated (principle of minimum energy) at this stage but can be easily related to the weak form of (1), see poster. Due to (2), $\bar{\Pi}$ is to be minimized with respect to ξ.

The order reduction enters this context when we seek the fluctuations within a low-dimensional subspace of the FE space V_{FE},

$$\dim\left(\mathrm{span}\left(\mathcal{L}\right)\right) = N \ll N_{\text{FE}} = \dim\left(V_{\text{FE}}\right).$$

In a discrete setting, (2) becomes

$$\underline{F}(\underline{x},t) \;=\; \bar{\underline{F}}(t) \;+\; \underline{\underline{L}}(\underline{x})\,\underline{\xi}(t) \qquad\qquad \underline{\xi}(t)\in\mathbb{R}^N,\; \underline{\underline{L}}(\underline{x})\in\mathbb{R}^{9\times N},\; \left\langle \underline{\underline{L}} \right\rangle = \underline{0}$$

where the columns of the matrix $\underline{\underline{L}}(\underline{x})$ are N reduced basis vectors which are yet to be determined. Straight-forward differentiation of (3) leads to the residual

$$\underline{r} = \frac{\partial \langle W \rangle}{\partial \underline{\xi}} \;=\; \left\langle \frac{\partial W}{\partial \underline{F}} \frac{\partial \underline{F}}{\partial \underline{\xi}} \right\rangle \;=\; \left\langle \underline{P}^{\mathsf{T}} \underline{\underline{L}} \right\rangle \;\stackrel{!}{=}\; \underline{0} \;\in \mathbb{R}^N \tag{4}$$

and its Jacobian

$$\underline{\underline{J}} = \frac{\partial^2 \langle W \rangle}{\partial \underline{\xi} \partial \underline{\xi}} \;=\; \left\langle \left(\frac{\partial \underline{F}}{\partial \underline{\xi}} \right)^{\mathsf{T}} \frac{\partial^2 W}{\partial \underline{F} \partial \underline{F}} \frac{\partial \underline{F}}{\partial \underline{\xi}} \right\rangle \;=\; \left\langle \underline{\underline{L}}^{\mathsf{T}}\, \underline{\underline{C}}\, \underline{\underline{L}} \right\rangle \;\in \mathbb{R}^{N\times N} \tag{5}$$

which suffice for the application of many optimization routines, e.g. Quasi-Newton schemes.

2.2 Homogenized material response

Given $\bar{\underline{F}}$ as an input, the presented model first finds the corresponding, unique coefficients $\underline{\xi}$ for the deformation gradient fluctuations minimizing (3) in the discrete chosen setting. With these at hand, the outputs of interest can be computed:

$$\bar{\underline{P}} = \left\langle \frac{\partial W}{\partial \underline{F}}\Big|_{\underline{F}(\underline{\xi})} \right\rangle, \qquad\qquad \bar{\underline{\underline{C}}} = \left\langle \underline{\underline{C}} \right\rangle - \left\langle \underline{\underline{C}}\, \underline{\underline{L}} \right\rangle \underline{\underline{J}}^{-1} \left\langle \underline{\underline{L}}^{\mathsf{T}} \underline{\underline{C}} \right\rangle$$

Note that $\frac{\partial W}{\partial \underline{F}}\big|_{\underline{F}(\underline{\xi})} = \underline{P}(\underline{\xi})$ can be reused from (4), and $\underline{\underline{J}}$ from (5) might also not need to be reassembled. It is further noteworthy that the effective stiffness tensor's matrix representation $\bar{\underline{\underline{C}}}$ is inherently symmetric.

2.3 Error evaluation

The quality of any ROM with output $\underline{P}$ can be assessed, e.g., by computing the vector of nodal residual forces $\underline{f}$ as in the FEM, i.e.

$$\underline{f} = \sum_{e=1}^{n_e} \underline{\underline{L}}^e \int_{\Omega_0^{\mathrm{e}}} \left(\underline{\underline{B}}^{\mathrm{e}}_{\mathrm{F}} \right)^{\mathsf{T}} \underline{P}\, \mathrm{d}V$$

where (as in standard FE literature) $\underline{\underline{B}}^{\mathrm{e}}_{\mathrm{F}}$ denotes the e^{th} element's B-matrix corresponding to $\mathbf{F}$ and $\underline{\underline{L}}^e$ is the element's local to global node mapping matrix. Then the accuracy can be judged the same way as in the FEM, e.g. by the same tolerances, without actually solving an FE problem. This also highlights that no additional discretization error is introduced by the ROM. One could relate $\underline{f}$ to the error in the displacements $\underline{x} - \underline{X}$ using the theorem of Lax and Milgram. Crucial at this point is the generally unknown coercivity constant.

2.4 Algebraic constraint

The minimization problem (3) neglects the algebraic constraint $J > 0$ which is a physical restriction on the deformation. Violation of this must be avoided by all means since it would mean unphysical self-penetration of matter and cause numerical failure. Unfortunately this is sometimes the case. While there is a range of methods to solve this problem for the FEM (of which mixed finite elements and a decrease of the load increment are most prominent), such methods need to be adapted to or developed newly for the ROM. As a first step, we investigate the influence of simply excluding all integration points with $J < 0$ from Ω_0, i.e. restrict the volume averaging operator:

$$\langle \bullet \rangle\,|_{J>0} = \frac{1}{|\Omega_{J>0}|} \int_{\Omega_{J>0}} \bullet\, \mathrm{d}V \qquad \text{with} \quad \Omega_{J>0} = \{\mathbf{X} \in \Omega_0 \,|\, J(\mathbf{X}) > 0\}$$

3 Sampling and the offline phase

Until now the RB was assumed to be given in the form of $\underline{\underline{L}}$. In this work, it is identified by means of a classic POD on a set of $M \gg N$ FEM-precomputed snapshots of the deformation gradient fluctuations $\underline{F}^{(\mathrm{i})}_{\mathrm{fluct}} = \underline{F}^{(\mathrm{i})} - \bar{\underline{F}}^{(\mathrm{i})}$, $i \in 1, \dots, M$ (in the "offline" phase). The crux at this stage is how to choose the prescribed macroscopic loads $\bar{\underline{F}}^{(\mathrm{i})} \leftrightarrow \bar{\mathbf{F}}^{(\mathrm{i})}$ in order to both sample as much as possible of the $\bar{\mathbf{F}}$-space and not invest overly large amounts of computational resources. The latter point can easily render a whole ROM unrealistic for real-world problems, e.g. a uniform nine-dimensional "grid" of the components of $\bar{\mathbf{F}}$ is out of question. Inspired by many classic works on Lie-groups and their relationship to continuum mechanics, and by the additive decomposition of the hyperelastic energy $W(\mathbf{F}) = U(J) + \psi(\tilde{\mathbf{F}})$ for the microscopic constituents, we propose to sample the space of symmetric, isochoric, positive definite, macroscopic deformation gradients "centered" around the identity matrix by means of the matrix exponential map:

$$\exp : \ \{\mathbf{T} \in \mathbb{R}^{3\times 3} \,|\, \mathbf{T} = \mathbf{T}^{\mathsf{T}}, \mathrm{tr}\,(\mathbf{T}) = 0\} = \mathcal{T} \ni \mathbf{T} \ \mapsto \ \sum_{k=0}^{\infty} \frac{\mathbf{T}^k}{k!}$$

Here, $\mathcal{T}$ is the five-dimensional tangent space of the nonlinear manifold of symmetric and positive definite $\bar{\tilde{\mathbf{F}}}$. Some samples are chosen along certain directions $\mathbf{T} \in \mathcal{T}$ by $\exp(t_i \mathbf{T}) = \bar{\tilde{\mathbf{F}}}^{(i)}$, $t_i \in [0, t_{\max}]$. Additionally, the remaining dimensions of the space of all possible $\bar{\mathbf{F}}$ need to be treated. For instance pure volumetric $\bar{\mathbf{F}} = \mathrm{diag}(\bar{J}^{1/3})$ boundary conditions need to be included in the sampling set. This procedure has already yielded promising results and is also subject to ongoing research.

Conclusions

An evidentially efficient ROM is introduced, showing speedups in the order of 10^1-10^2 compared to the FEM. The accuracy is competitive, increases monotonically if the RB is enlarged, and can be quantified online. Modifications of the error indication are discussed. In order to decrease the computational offline costs to a manageable level, a new sampling strategy is proposed.

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