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Variational sensitivity analysis in the scope of multiscale problems

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Micro Abstract
The combination of methods for shape optimisation with different established approaches for analysis and simulation of complex heterogeneous materials on multiple scales based on numerical homogenisation techniques opens a remarkable range of applications introducing design variables, objective functions and constraints on different scales. To design micro-structures, the essential steps for sensitivity analysis on multiple scales will be outlined and accentuated by illustrative examples.

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Introduction

Environments for numerical homogenisation and FE^2 techniques are still a challenging area. Nevertheless, their major benefit is the ability to analyse complex mechanical problems with heterogeneous material behaviour on different scales. During the past two decades, several authors and groups published their long and ongoing work and their experiences on this topic in several journals and books, see [3, 5–8] just to name a few. Within all presented frameworks, the choice of *representative volume elements* (RVE), the choice of appropriate boundary conditions and the determination of effective or homogenised parameters, i.e. of effective stresses $\overline{\mathbf{P}}$ and material properties $\overline{\mathbb{A}}$ in Eq. (1), are essential

$$\overline{\mathbf{P}} = \frac{1}{\mathcal{V}} \int_\Omega \mathbf{P} \, \mathrm{d}\Omega = \frac{1}{\mathcal{V}} \int_\Gamma \boldsymbol{t} \otimes \boldsymbol{X} \, \mathrm{d}\Gamma, \qquad \overline{\mathbb{A}} = \frac{\partial \overline{\mathbf{P}}}{\partial \overline{\mathbf{F}}}. \tag{1}$$

Incorporation of this powerful methods for analysis of boundary value problems (BVP) on multiple scales (MSA) within frameworks for structural optimisation (SO) allows to design materials and microstructures, and to tailor macroscopic applications to their special requirements. Close attention has to be paid to the integrated design sensitivity analysis (DSA) due to its key role for accurate and efficient simulations, and also due to its potential for predictions.

1 Numerical homogenisation

The presented work is primarily based on the approach proposed in [3, 5], where the authors refer a finite dimensional minimisation problem with an averaged energy $\overline{W}$, cf. Eq. $(2)_1$, and a discrete *Lagrange functional* $\overline{W}_\mathrm{C}$, cf. Eq. $(2)_2$, for alternative boundary conditions $\mathrm{C} = (D), (P), (S)$, i.e. linear or periodic displacements or uniform tractions on the boundary of the chosen RVE in terms of appropriate boundary condition matrices $\mathcal{A}_\mathrm{C}$ and $\mathcal{B}_\mathrm{C}$

$$\overline{W}(\boldsymbol{u}) = \frac{1}{\mathcal{V}} \int_\Omega W(\boldsymbol{F}; \boldsymbol{X}) \, \mathrm{d}\Omega, \quad \overline{W}_\mathrm{C}(\overline{\boldsymbol{F}}, \overline{\boldsymbol{X}}) = \inf_{\boldsymbol{u}} \sup_{\boldsymbol{\lambda}_\mathrm{C}} \{ \overline{W}(\boldsymbol{u}) - \boldsymbol{\lambda}_\mathrm{C} \left[\mathcal{A}_\mathrm{C} \, \boldsymbol{u}_\mathrm{b} - \mathcal{B}_\mathrm{C} \, (\overline{\boldsymbol{F}} - \boldsymbol{I}) \right] \}. \tag{2}$$

This saddle point problem can be solved using a standard Newton method, where variations with respect to state variables $(\boldsymbol{u}_\mathrm{i}, \boldsymbol{u}_\mathrm{b})$ and the *Lagrange multiplier* $\boldsymbol{\lambda}_\mathrm{C}$ are necessary. Here, the indices (i, b) partition several quantities in inner values and values on the boundary of the referred domain. The obtained equilibrium state allows the computation of effective stresses $\overline{\boldsymbol{P}}_{\mathrm{C}}$ and tangent moduli $\overline{\boldsymbol{A}}_{\mathrm{C}}$ in matrix form by

$$\overline{\boldsymbol{P}}_{\mathrm{C}} = \partial_{\overline{\boldsymbol{F}}} \overline{W}_{\mathrm{C}} = \mathcal{B}_{\mathrm{C}}^{T} \boldsymbol{\lambda}_{\mathrm{C}}, \qquad \overline{\boldsymbol{A}}_{\mathrm{C}} = \partial^{2}_{\overline{\boldsymbol{F}}\,\overline{\boldsymbol{F}}} \overline{W}_{\mathrm{C}} = \partial_{\overline{\boldsymbol{F}}} \overline{\boldsymbol{P}}_{\mathrm{C}} = \mathcal{B}_{\mathrm{C}}^{T} \frac{\partial \boldsymbol{\lambda}_{\mathrm{C}}}{\partial \overline{\boldsymbol{F}}} = \mathcal{B}_{\mathrm{C}}^{T} \overline{\boldsymbol{K}}\, \mathcal{B}_{\mathrm{C}}. \tag{3}$$

Here, the condensed matrix $\overline{\boldsymbol{K}}$ in terms of degrees of freedom on the boundary of the RVE is used, see [5] for details and exact representations. The solution of the overall coupled macro-micro BVP requires the solution of the macroscopic residual (4) in terms of resulting effective parameters $\overline{\mathbf{P}}$ and external macroscopic loads $\overline{F}(\overline{\boldsymbol{\eta}})$

$$\overline{R}(\overline{\boldsymbol{u}}, \overline{\boldsymbol{X}}, \boldsymbol{u}, \boldsymbol{X}; \overline{\boldsymbol{\eta}}) = \int_{\overline{\Omega}} \overline{\mathbf{P}} : \overline{\mathbf{F}}'_{\overline{u}}(\overline{\boldsymbol{\eta}})\, \mathrm{d}\overline{\Omega} - \overline{F}(\overline{\boldsymbol{\eta}}) = 0. \tag{4}$$

In general, the solution of the macroscopic BVP requires variations of the residual $\overline{R}$ with respect to the state parameters $(\overline{\boldsymbol{u}}, \boldsymbol{u})$ for structural analysis and with respect to design parameters $(\overline{\boldsymbol{X}}, \boldsymbol{X})$ for structural optimisation. Furthermore, the variational relation in Eq. (5) has to be fulfilled for any arbitrary state or design variation to guarantee equilibrium

$$\overline{R}' = \overline{R}'_{\overline{u}} + \overline{R}'_{\overline{X}} + \overline{R}'_{u} + \overline{R}'_{X} = 0. \tag{5}$$

This total variation $\overline{R}'$ contains variations of effective stresses $\overline{\mathbf{P}}$ in each partial term and results in well-known tangent operators, i.e. stiffness tangent operator for structural analysis and pseudo load tangent operator for structural optimisation. All details on variational sensitivity analysis on single scales, on variations of kinematical quantities or further quantities from continuum mechanics, and explicit representations of pseudo loads matrices can be found in [1, 2, 4].

2 Sensitivity of effective stresses

The essential quantity $\overline{\mathbf{P}}$ in the homogenisation scheme and especially its variation with respect to state and design variables has to be investigated. It is sufficient to consider relations for sensitivity analysis on single scales, which are presented in [1, 2, 4] in detail. In computations, the effective stresses $\overline{\boldsymbol{P}}_{\mathrm{C}}$ in Eq. $(3)_1$ depend on the constant boundary conditions matrix $\mathcal{B}_{\mathrm{C}}$ and the Lagrange multiplier $\boldsymbol{\lambda}_{\mathrm{C}}$. Therefore, the variation of effective stresses $\overline{\boldsymbol{P}}_{\mathrm{C}}$ follows to

$$(\,\overline{\boldsymbol{P}}_{\mathrm{C}}(\boldsymbol{\lambda}_{\mathrm{C}}))' = \frac{\partial \overline{\boldsymbol{P}}_{\mathrm{C}}}{\partial \boldsymbol{\lambda}_{\mathrm{C}}} (\boldsymbol{\lambda}_{\mathrm{C}})' = \mathcal{B}_{\mathrm{C}}^{T} \left[(\boldsymbol{\lambda}_{\mathrm{C}})'_{u} + (\boldsymbol{\lambda}_{\mathrm{C}})'_{X} \right]. \tag{6}$$

In accordance to the concept in [5], the Lagrange multiplier $\boldsymbol{\lambda}_{\mathrm{C}}$ corresponds to resulting reaction forces on the boundary of the considered domain and as a consequence, relation $(7)_1$ holds true. The total variation of the Lagrange multiplier $\boldsymbol{\lambda}_{\mathrm{C}}$ with respect to state and design parameters results to Eq. $(7)_2$ and requires partial variations of the residual $\boldsymbol{R}_{\mathrm{b}}$ on the boundary

$$\boldsymbol{\lambda}_{\mathrm{C}} = \boldsymbol{R}_{\mathrm{b}}^{\mathsf{ext}} = \boldsymbol{R}_{\mathrm{b}}^{\mathsf{int}}, \qquad (\boldsymbol{\lambda}_{\mathrm{C}})' = (\boldsymbol{\lambda}_{\mathrm{C}})'_{u} + (\boldsymbol{\lambda}_{\mathrm{C}})'_{X} = (\boldsymbol{R}_{\mathrm{b}}^{\mathsf{ext}})' = (\boldsymbol{R}_{\mathrm{b}}^{\mathsf{int}})' = (\boldsymbol{R}_{\mathrm{b}}^{\mathsf{int}})'_{u} + (\boldsymbol{R}_{\mathrm{b}}^{\mathsf{int}})'_{X}. \tag{7}$$

Remark 2.1 *The total variation of a quantity $f(\boldsymbol{u}, \boldsymbol{s})$ with respect to design $\boldsymbol{s}$ is determined by*

$$f' = \frac{\partial f}{\partial \boldsymbol{u}} \delta \boldsymbol{u} + \frac{\partial f}{\partial \boldsymbol{s}} \delta \boldsymbol{s} = \left(\frac{\partial f}{\partial \boldsymbol{u}}\ \boldsymbol{S} + \frac{\partial f}{\partial \boldsymbol{s}} \right) \delta \boldsymbol{s} \tag{8}$$

with the sensitivity matrix $\boldsymbol{S} = -\boldsymbol{K}^{-1}\boldsymbol{P}$ being the sensitivity of the state variable $\delta \boldsymbol{u} = \boldsymbol{S} \delta \boldsymbol{s}$.

Equal to the partition of the state, design parameters can be partitioned using indices (I, B). Using defined subsets (i, b) and (I, B), all necessary quantities and relations can be separated

$$\boldsymbol{u} = \begin{bmatrix} \boldsymbol{u}_{\mathrm{i}} \\ \boldsymbol{u}_{\mathrm{b}} \end{bmatrix}, \delta \boldsymbol{u} = \begin{bmatrix} \delta \boldsymbol{u}_{\mathrm{i}} \\ \delta \boldsymbol{u}_{\mathrm{b}} \end{bmatrix}, \boldsymbol{X} = \begin{bmatrix} \boldsymbol{X}_{\mathrm{I}} \\ \boldsymbol{X}_{\mathrm{B}} \end{bmatrix}, \delta \boldsymbol{X} = \begin{bmatrix} \delta \boldsymbol{X}_{\mathrm{I}} \\ \delta \boldsymbol{X}_{\mathrm{B}} \end{bmatrix}, \tag{9}$$

and a partitioned representation of the physical residual (cf. Eq. $(10)_1$) and of its variation or linearised form (cf. Eq. $(10)_2$) can be stated

$$\boldsymbol{R}(\boldsymbol{u},\boldsymbol{X};\boldsymbol{\eta}) = \begin{bmatrix} \boldsymbol{R}_\mathrm{i}(\boldsymbol{u}_\mathrm{i},\boldsymbol{u}_\mathrm{b},\boldsymbol{X}_\mathrm{I},\boldsymbol{X}_\mathrm{B};\boldsymbol{\eta}) \\ \boldsymbol{R}_\mathrm{b}(\boldsymbol{u}_\mathrm{i},\boldsymbol{u}_\mathrm{b},\boldsymbol{X}_\mathrm{I},\boldsymbol{X}_\mathrm{B};\boldsymbol{\eta}) \end{bmatrix}, \qquad \boldsymbol{R}' = \begin{bmatrix} \boldsymbol{R}'_\mathrm{i} \\ \boldsymbol{R}'_\mathrm{b} \end{bmatrix} = \begin{bmatrix} (\boldsymbol{R}_\mathrm{i})'_u + (\boldsymbol{R}_\mathrm{i})'_X \\ (\boldsymbol{R}_\mathrm{b})'_u + (\boldsymbol{R}_\mathrm{b})'_X \end{bmatrix}. \tag{10}$$

Here, the partial variations of the partitioned residual $\boldsymbol{R}_\mathrm{i}, \boldsymbol{R}_\mathrm{b}$ with respect to the partitioned state $(\boldsymbol{u}_\mathrm{i}, \boldsymbol{u}_\mathrm{b})$ and the partitioned design $(\boldsymbol{X}_\mathrm{I}, \boldsymbol{X}_\mathrm{B})$ are provided by the sub-matrices in Eq. (11).

$$\boldsymbol{R}'_u = \begin{bmatrix} (\boldsymbol{R}_\mathrm{i})'_u \\ (\boldsymbol{R}_\mathrm{b})'_u \end{bmatrix} = \begin{bmatrix} \boldsymbol{K}_\mathrm{ii} & \boldsymbol{K}_\mathrm{ib} \\ \boldsymbol{K}_\mathrm{bi} & \boldsymbol{K}_\mathrm{bb} \end{bmatrix} \begin{bmatrix} \delta\boldsymbol{u}_\mathrm{i} \\ \delta\boldsymbol{u}_\mathrm{b} \end{bmatrix}, \qquad \boldsymbol{R}'_X = \begin{bmatrix} (\boldsymbol{R}_\mathrm{i})'_X \\ (\boldsymbol{R}_\mathrm{b})'_X \end{bmatrix} = \begin{bmatrix} \boldsymbol{P}_\mathrm{iI} & \boldsymbol{P}_\mathrm{iB} \\ \boldsymbol{P}_\mathrm{bI} & \boldsymbol{P}_\mathrm{bB} \end{bmatrix} \begin{bmatrix} \delta\boldsymbol{X}_\mathrm{I} \\ \delta\boldsymbol{X}_\mathrm{B} \end{bmatrix}. \tag{11}$$

Application of Remark 2.1 to Eq. $(7)_2$ and referring the partitioned variations of the residual in Eq. (11), the partial variations of the residual on the boundary can be identified by

$$(\boldsymbol{R}^\mathsf{int}_\mathrm{b})'_u = \frac{\partial \boldsymbol{R}^\mathsf{int}_\mathrm{b}}{\partial \boldsymbol{u}} \delta\boldsymbol{u} = \boldsymbol{K}_\mathrm{bi}\,\delta\boldsymbol{u}_\mathrm{i} = \boldsymbol{K}_\mathrm{bi}\boldsymbol{S}_\mathrm{i}\,\delta\boldsymbol{X}, \qquad (\boldsymbol{R}^\mathsf{int}_\mathrm{b})'_X = \frac{\partial \boldsymbol{R}^\mathsf{int}_\mathrm{b}}{\partial \boldsymbol{X}}\,\delta\boldsymbol{X} = \boldsymbol{P}_\mathrm{b}\,\delta\boldsymbol{X}. \tag{12}$$

Finally, the explicit total variation of the Lagrange multiplier from Eq. $(7)_2$ can be expressed by

$$(\boldsymbol{\lambda}_\mathrm{C})' = (\boldsymbol{R}^\mathsf{ext}_\mathrm{b})' = (\boldsymbol{R}^\mathsf{int}_\mathrm{b})' = [\boldsymbol{K}_\mathrm{bi}\ \boldsymbol{S}_\mathrm{i}\ + \boldsymbol{P}_\mathrm{b}]\,\delta\boldsymbol{X}, \tag{13}$$

and is used for computations of required sensitivity information of effective stresses from Eq. (6).

3 Numerical investigations

In the context of multiscale optimisation problems, the sensitivity of reaction forces couples referred scales, i.e. it represents the sensitivity relation of the homogenisation condition. The advantage of presented relations in Eq. (12) and Eq. (13) is, that they hold true for optimisation problems on single scales in a similar manner, so that they can be used as constraints in usual optimisation problems on single scales. The purpose of the following example is to motivate the application of the sensitivity information of reaction forces from Eq. (13) and to discuss its influence on resulting effective stresses within the sensitivity analysis of multiscale optimisation problems. Therefore, the deformation mode $\overline{\boldsymbol{F}} = \begin{bmatrix}1.2 & 1.1 & 0.1 & 0.05\end{bmatrix}^T$ is utilised to evaluate the microstructure in Fig. 1 for periodic boundary conditions, i.e. $\mathrm{C} = (P)$, with arbitrarily chosen design variables $(a,b)^\mathrm{ini} = (0.75, 0.25)$ for the diameters. The target is to minimise the volume $J = V$ of the RVE and to control physical reaction forces $\boldsymbol{g} = \boldsymbol{F}_\mathrm{R} \le \boldsymbol{F}^\mathrm{max}_\mathrm{R}$ on the boundary. Moreover, defined side constraints $\boldsymbol{s}^\mathrm{l} = 0.1 \le \boldsymbol{s} \le 0.8 = \boldsymbol{s}^\mathrm{u}$ have to be fulfilled.

The mathematical optimisation algorithm (SQP) used 28 iterations to obtain a minimum value for the objective (reduction by approximately 27%). In parallel, the incorporation of reaction forces as constraints gives the advantage to reduce them by approximately 25% compared to the initial design and has a direct influence on the reduction of effective stresses, cf. Eq. (14)

$$\overline{\boldsymbol{P}}^\mathrm{ini}_P = \begin{bmatrix}26.14 & 10.32 & 5.59 & 5.36\end{bmatrix}^T, \qquad \overline{\boldsymbol{P}}^\mathrm{opt}_P = \begin{bmatrix}15.62 & 6.80 & 2.56 & 2.43\end{bmatrix}^T. \tag{14}$$

When it comes to local stresses in the chosen RVE as quantities of interest, Fig. 1 proves, that in this example the maximum amplitude of local *Von-Mises* stresses can be reduced too, i.e. $\sigma^\mathrm{ini}_\mathrm{max} = 960.85$ and $\sigma^\mathrm{opt}_\mathrm{max} = 509.55$. The final design parameters result to $(a,b)^\mathrm{opt} = (0.80, 0.60)$. All discussed results, i.e. for the objective, the constraint and the local stress distribution for initial and optimised design, are shown in Fig. 1. The incorporation of the sensitivity information for reaction forces is necessary to be able to control the homogenised and effective parameters on the macroscale. This statement holds true for any other choice of microscopic material representation or RVE. In this example, the possible number of design variables is small. Nevertheless, when it comes to multiscale optimisation problems, the amount of possible design parameters might become enormous due to arbitrary design parameters on the macroscale and several combinations of design parameters for the design of microstructures.

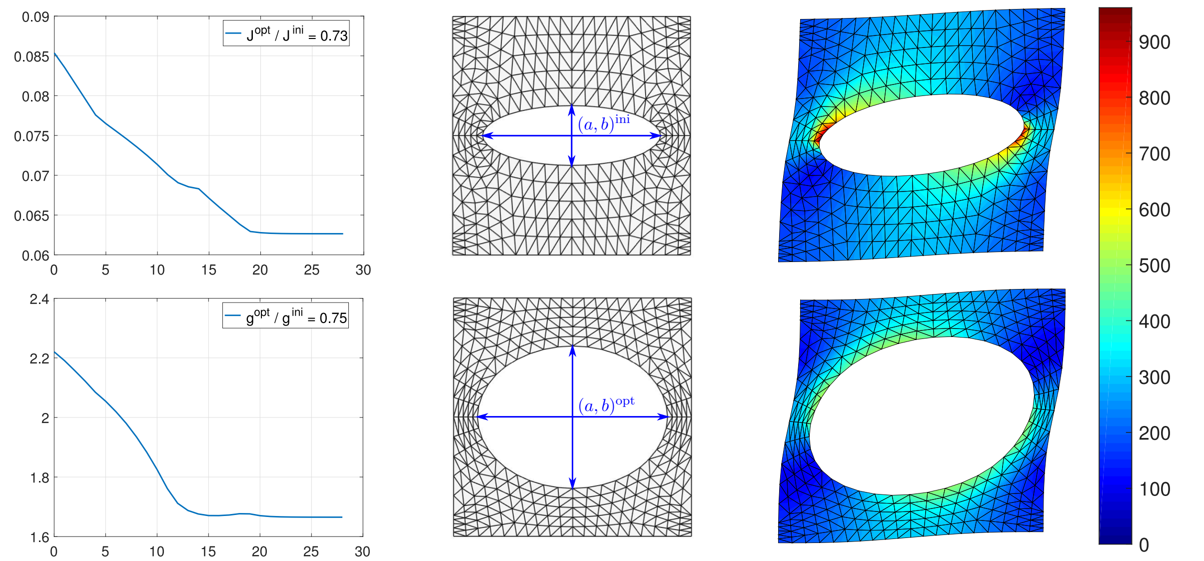

Figure 1. *Left:* Optimisation results (objective J and constraint g) over iterations. *Middle:* Initial (top) and optimised (bottom) design. *Right:* Von-Mises stress distribution for initial (top) and optimal (bottom) design.

Conclusions

Formulations of multiscale methods, based on homogenisation in terms of quantities on the boundary of referred domains, can be enhanced by presented elements from variational sensitivity analysis. This extension is predestinated for predictions about the behaviour on different scales, and especially for improvements and design of underlying micro-materials and structures.

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