Optimal design of unit-cell based programmable materials

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An optimal design for a programmable material based on an array of unit-cells is established. A programmable material behavior is achieved by using unit-cells with complex and adjustable features arising from the inner structure of each cell. This type of materials has the potential of replacing the functionality of entire systems consisting of sensors and actuators, provided that an optimal inner structure is given. In this paper the multiscale optimization problem and a solution strategy are presented. An efficient data driven method is used for the solution of the macroscopic boundary value problem. Finally, an example of an optimized parameter distribution for a unit-cell based material is shown.

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1 Multiscale optimization problem

A programmable material \( \hat{\Omega} \) can be considered as an array of functional unit-cells \( \tilde{\Omega}(\alpha) \) as shown in Fig. 1 which are connected to each other. The design parameters \( \alpha(X) \) represent angles, lengths and thicknesses inside the cells which are used to adjust the mechanical behavior of a cell. By combining a huge amount of unit-cells (e.g. \( 100^3 \ldots 1000^3 \)), the array \( \hat{\Omega} \) can be interpreted as one material which is described by a constitutive law

\[
\hat{S} = 2 \frac{\partial \hat{W}(\hat{C}, \alpha)}{\partial \hat{C}}
\]

where \( \hat{S} \), \( \hat{W} \) and \( \hat{C} \) are the second Piola-Kirchhoff stress tensor, the macroscopic internal energy density and the right Cauchy-Green deformation tensors, respectively. The multiscale optimization problem reads as

\[
\min_{\alpha} ||u(\alpha) - u_\ast|| \quad \text{on} \quad \hat{\Gamma}_\ast
\]

s.t.

\[
\text{Div}(\hat{F} \hat{S}) = 0 \quad \text{in} \quad \hat{\Omega}, \quad u = u_d \quad \text{on} \quad \hat{\Gamma}_d, \quad \sigma \cdot n = \hat{t} \quad \text{on} \quad \hat{\Gamma}_n.
\]

Eq. (2) is the optimization problem with constraints imposed by the macroscopic mechanical boundary value problem (BVP) Eq. (3). In the BVP, the first term is the balance of momentum and the subsequent expressions are the Dirichlet and Neumann boundary conditions, respectively.

The design variables \( \alpha \) in Eq. (1) connect the macroscopic material scale to the microscopic scale of the unit-cell as the macroscopic material behavior is mainly determined by microscopic geometry parameters \( \alpha \). Hence, in order to solve the

Fig. 1: Multiscale optimization problem: \( \bullet \) denotes a macroscopic quantity, \( \circ \) a microscale quantity. The array of unit-cells \( \hat{\Omega} \) is subjected to Dirichlet and Neumann boundary conditions on \( \hat{\Gamma}_d \) and \( \hat{\Gamma}_n \). The objective function \( u_\ast \) is defined on \( \hat{\Gamma}_\ast \). The unit-cells \( \tilde{\Omega} \) are characterized by geometric design parameters \( \alpha \) such a joint thickness \( \hat{t} \). Various types of cells can be used in the array, interconnected through their boundaries \( \tilde{\Gamma}_d \). Here a unit-cell with potential inner contact under horizontal or vertical compression is shown. Areas with potential inner contact are denoted by \( \tilde{\Gamma}_c \).
macroscopic BVP, the mechanical response of the unit-cell has to be calculated. This introduces the microscopic BVP which reads as follows:

\[
\text{Div}(\tilde{F}\tilde{S}) = 0 \quad \text{in} \quad \tilde{\Omega}(\alpha) \\
u = \hat{u} \quad \text{on} \quad \tilde{\Gamma}_{d}, \quad \sigma \cdot n = 0 \quad \text{on} \quad \tilde{\Gamma}_{n}, \quad g_{n}(u) \geq 0 \quad \text{on} \quad \tilde{\Gamma}_{c}.
\] (4)

The gap function \(g_{n}\) ensures that no self-penetration on \(\tilde{\Gamma}_{c}\) takes place. The constitutive model on the microscale is described by a nonlinear potential

\[
\tilde{S} = 2\frac{\partial W(\tilde{C},\beta)}{\partial \tilde{C}}
\] (5)
such as a Neo-Hookean law where \(\beta\) are material parameters. In Eq. (4) the boundary condition \(\hat{u}\) is calculated by imposing a macroscopic deformation

\[
\hat{u}(X) = (\hat{F} - 1)X + u_{p} = (\hat{C}^{1/2} - 1)X + u_{p} \quad \text{on} \quad \tilde{\Gamma}_{d}
\] (6)

where \(u_{p}\) is a periodic function over \(\tilde{\Omega}\).

### 2 Solution and results

The optimization problem in Eq. (2) is solved using an iterative gradient based optimization scheme according to [1]. In every iteration, the multiscale BVP Eq. (3) has to be solved and therefore a fast solution of this problem is needed. Further, the derivative of the unit-cell’s macroscopic behavior w.r.t. the design variables is required. Therefore a data based solution approach as proposed by [2] is chosen for Eq. (3).

A database \(D : \mathbb{R}^{n_{\alpha}} \times \mathbb{R}^{n_{C}} \to \mathbb{R}^{6}\) is precomputed which maps a specific geometry variant \(\alpha^{i}\) and macroscopic loadcase \(C^{j}\) to a macroscopic stress \(\tilde{S}\). Here, \(n_{\alpha}\) and \(n_{C}\) are the number of design variants and loadcases. The discrete values \(D_{i,j}\) are interpolated by a continuous and differentiable function s.t. \(D(\alpha^{i},C^{j}) \approx D_{i,j}\). The interpolation function is used as a surrogate model for the unit-cells’ mechanical behavior. Further, it allows to calculate the derivative of the material behavior w.r.t. \(\alpha\) which is used in the optimization. For each point \(D_{i,j}\) a FE simulation is performed to solve Eq. (4), which represents a large computational effort. However due to precomputing the database, parallelization is very easy and the multiscale simulation is very fast.

As an example, the problem shown in Fig. 1 is solved. The array consists of \(20 \times 10 \times 1\) cells from the type that is also shown in Fig. 1. It has a variable joint thickness \(t_{g}\) which influences the stiffness of the cell. The objective function is a given target deformation on the upper boundary under a sideways loading. Fig. 2 shows the optimized distribution of the design variable. In Fig. 3 the convergence of the scheme can be seen. The objective function and the given computed data match very well. Our proposed scheme converged after approx. 20 iterations, which again shows the need for a fast solution of the macroscopic BVP.

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