Optimal Experimental Design to Identify the Average Stress-Strain Response in Short Fiber-Reinforced Plastics

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We show how to use optimal experimental design methods for the parameter identification of short fiber reinforced plastic (SFRP) materials. The experimental data is given by computer simulations of representative volume elements (RVE) of the SFRP material. The experiments are designed such that a minimal number of RVE simulations is required and that the model response attains a minimal variance for a class of strains and fiber orientations.

1 Modeling of SFRP Materials

The governing constitutive law of an SFRP material in the linear elastic case is derived by the so-called averaging procedure of Tucker [1] applied to the constitutive law of a unidirectional composite (transversely anisotropic in the fiber direction):

\[ C_{\text{sfrp}}(\varepsilon, A) : \varepsilon = c_1 \varepsilon + c_2 \text{tr}(\varepsilon) I + c_3 (A \text{tr}(\varepsilon) + (A : \varepsilon) I) + c_4 (A \varepsilon + \varepsilon A) + c_5 A : \varepsilon , \]

where \( A \) is the second and \( \hat{A} \) is the fourth moment of the fiber orientation distribution. In order to keep the dimensionality of the problem reasonable, we compute \( \hat{A} \) from the second moment \( A \) using the ORW3 closure [2]. The parameter vector \( c := (c_1, \ldots, c_5)^T \) contains material constants, which depend on the material parameters of the fiber and matrix material, as well as the volume fraction and aspect-ratio of the fibers.

2 Parameter Identification Problem

Given the average stresses \( \sigma_i := (\sigma_{i,j}) \in \text{Sym}(3) \), \( i = 1, \ldots, n_{\exp} \) of \( n_{\exp} \) experiments (RVE simulations), each performed with the prescribed average strain \( \varepsilon_i \) and the moments of the fiber orientation distribution \( A_i \) the goal is to identify the parameter vector \( c \) in (1) which minimizes the sum of squared residuals

\[ s(c) := \frac{1}{2} \sum_{i=1}^{n_{\exp}} \|C_{\text{sfrp}}(c, A_i) : \varepsilon_i - \sigma_i\|^2_F \longrightarrow \min. \]

An optimal solution of this least-squares problem satisfies the normal equation

\[ \mathcal{I} c = J^T y \quad \text{with} \quad \mathcal{I} := J^T J \in \mathbb{R}^{5 \times 5}. \]

\( \mathcal{I} \) denotes the Fisher information matrix and \( J \) denotes the Jacobian of the residual in (2). \( y \) is a vector containing the vectorized experimental data \( \sigma_i \). A priori it is not clear how to choose the design variables \( \varepsilon_i \) and \( A_i \) as well as the number of experiments \( n_{\exp} \) such that \( \mathcal{I} \) becomes positive definite and, in a sense, as large as possible. Computing the complete stiffness matrix first and then identifying the parameters from there is possible (c.f. [3]), however this is a rather costly procedure.

3 Optimal Experimental Design Problem

Due to the discrete nature of computer experiments, the vector of experimental data \( y \) usually contains errors, which do not change if we perform exactly the same experiment again. However, the experimental setup (defined through the design variables \( A_i, \varepsilon_i \)) determines the amplification of these errors in the determined parameters \( c \). Since the sign and magnitude of these errors is a priori not known, we assume that each component of \( \varepsilon_i \) and \( A_i \) as well as the number of experiments \( n_{\exp} \) contains random errors and that \( y \) follows a multivariate Gaussian distribution \( y \sim \mathcal{N}(\bar{y}, \Sigma_y) \) with mean value \( \bar{y} \) and covariance \( \Sigma_y \). The variance of the parameters is then given by

\[ \Sigma_c := \sigma_y^2 \mathcal{I}^{-1}. \]

And the variance of the model response (evaluated and averaged over all possible rank one strains of unity norm and rank one fiber orientation moments) is given by

\[ \Sigma_\bar{y} = \sigma_y^2 W \mathcal{I}^{-1} \quad \text{with} \quad W = \frac{1}{15} \begin{pmatrix} 15 & 15 & 10 & 10 & 3 \\ 15 & 45 & 30 & 10 & 5 \\ 10 & 30 & 34 & 16 & 8 \\ 10 & 10 & 16 & 16 & 6 \\ 3 & 5 & 8 & 6 & 3 \end{pmatrix}. \]

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The solutions of (3) for \( n_{\text{exp}} = 1 \) are given in Table 1. For Design I we have \( \text{rank}(A_1) = 2 \), i.e., a planar fiber distribution turns out to be optimal. Design II requires two experiments with unidirectional fiber orientations (\( \text{rank}(A_1) = 1 \)). The rank 1 solutions are generally more favorable as they allow more densely packed fibers and more efficient/simple computations as well as experimental setups (i.e., for tensile specimens). When we use the quadratic closure instead of the ORW3 closure no parameter identification is possible due to a rank-deficient Jacobian \( J \). For Design I this is the case if one eigenvalue of \( A_1 \) has a multiplicity of 2. For Design II, a variation of \( A_1 \) has only small influence on the objective, so it can be chosen more or less arbitrarily. Looking at Figure 1 it seems that there are multiple local minimizers. However, since we restricted the moments to the triangle \( 0 \geq a_1 \geq a_2 \geq a_3 \), these symmetric solutions disappear and there is only one solution for \( A_1 \) and \( A_2 \). The optimal \( A_i \) imply certain symmetries for \( \varepsilon \), which do not change the objective. Therefore all optimal solutions are global optimal.

Further experiments revealed that Design II is a robust choice for the parameter identification. For \( n_{\text{exp}} > 2 \) the designs are clustering (due the assumption of uncorrelated noise) and do not reduce the optimal objective function value any further. More details are available in the preprint [4], submitted to CMAME.

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**References**

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