



Relating Local Field Fluctuations in Composites with the Sensitivity of Their Effective Response to Constitutive Parameters: An Identification Framework for Elastic and Viscoelastic Materials

Robin Valmalette, Cédric Bellis, Christian Hochard, Noël Lahellec

► To cite this version:

Robin Valmalette, Cédric Bellis, Christian Hochard, Noël Lahellec. Relating Local Field Fluctuations in Composites with the Sensitivity of Their Effective Response to Constitutive Parameters: An Identification Framework for Elastic and Viscoelastic Materials. *International Journal of Solids and Structures*, 2025, 321, pp.113580. <10.1016/j.ijsolstr.2025.113580>. <hal-05189041v2>

HAL Id: hal-05189041

<https://hal.science/hal-05189041v2>

Submitted on 8 Aug 2025

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



HAL Authorization

Relating local field fluctuations in composites with the sensitivity of their effective response to constitutive parameters: An identification framework for elastic and viscoelastic materials.

Robin Valmalette^a, Cédric Bellis^{a,*}, Christian Hochard^a, Noël Lahellec^a

^a*Aix Marseille Univ, CNRS, Centrale Med, LMA UMR 7031, 4 impasse Nikola Tesla, Marseille, 13453, France*

Abstract

In the study of composite materials, accurately characterizing the individual properties of constituents is essential but often challenging due to the possible unavailability of raw materials and the complexity of conducting microscale experiments. Inverse homogenization offers a compelling solution by enabling the extraction of microscale properties directly from macroscale experiments, despite being an ill-posed problem. This study focuses on identifying unknown constitutive parameters by minimizing a cost function that measures the discrepancy between actual composite response data and the predicted homogenized behaviour based on candidate parameters. To tackle these optimization problems, both first and second-order gradient-based minimization schemes are employed. This requires evaluating the sensitivity of a composite's effective response to its constitutive parameters, which is related to local fluctuations in solution fields of elementary cell problems. To so do, first and second-order derivatives of macroscopic stress and effective energy potential are obtained in a general setting, including nonlinear behaviours. Sensitivity maps are computed to gain local information within the representative volume element. The methodology involves repeatedly solving cell problems, efficiently achieved using FFT-based full-field simulations for periodic composites. It is implemented in two test cases involving fiber-reinforced composites to identify hard-to-measure parameters: elastic properties of fibers and viscoelastic properties of the matrix. The latter case uses the Laplace–Carson transform to extend the method to viscoelastic materials. The targeted constitutive properties are successfully identified, and sensitivity analyses assess the effects of uncertainties on the identified parameters. The study provides guidelines for using this sensitivity-based approach in relevant situations.

Keywords: parameter identification, inverse homogenization, full-field simulations, multiscale methods, FFT-based homogenization, viscoelasticity

1. Introduction

The application of multiphase and multiscale composites in industrial applications is flourishing, reinforcing the need to understand and predict phenomena across multiple scales in materials. To study the behaviour of composite materials, micromechanical models and homogenization methods

*Corresponding author

Email addresses: valmalette@lma.cnrs-mrs.fr (Robin Valmalette), bellis@lma.cnrs-mrs.fr (Cédric Bellis), hochard@lma.cnrs-mrs.fr (Christian Hochard), lahellec@lma.cnrs-mrs.fr (Noël Lahellec)

can be used to predict their effective macroscopic responses from the knowledge of their microstructure and the material properties of their constituents. To take an example relevant to the present study, the measurement and modelling of the overall elastic properties of fibre-reinforced plastics are challenging given the complex failure mechanisms they can undergo, including matrix and fibre failures (Swolfs et al., 2015; Chen et al., 2019; Mishnaevsky and Brøndsted, 2008; Wang et al., 2020; Qing and Mishnaevsky, 2009; Merlette and Diani, 2025; Praud et al., 2021; Verpoest and Lomov, 2005).

Micromechanical homogenization models are based on a description of the microstructure and knowledge of the properties of the phases, which are used in a given homogenization scheme (using mean-field or full-field approaches). While advances in tomographic imaging and image processing have made microstructural data more easily accessible, determining the mechanical properties of the constituents remains challenging. Different factors contribute to these difficulties: First, the composite constituents may not be easily available as raw materials. Second, microscale experiments can be extremely difficult to carry out because of size constraints. For instance, carbon fiber are transversely isotropic with diameters around $7\text{ }\mu\text{m}$. In this case, microscale experiments are particularly challenging (Islam et al., 2020; Mounier et al., 2014); suppliers typically report only one of the five moduli, and the few available references often lack detail or do not report uncertainties (Soden et al., 1998). Because of the lack of data, some authors tend to consider parameters approximated from a few available references — which do not always match specifically the material they investigate — (Katouzian and Vlastakis, 2020; Gonçalves et al., 2022; Donadon et al., 2007; Goldberg et al., 2015; Blackketter et al., 1993; Miyagawa et al., 2005). Lastly, the manufacturing process itself can affect the properties of a *known* material, *e.g.* polymer in a neat matrix *vs.* polymer in a processed composite material (Gregory and Spearing, 2005; Breite et al., 2021; Ureña et al., 2005).

An alternative to in situ microscale experiments is the inverse homogenization approach, which aims at inferring microscale parameters directly from macroscale data for a given composite. Also referred to as reverse engineering or dehomogenization, this method can be formulated as a minimisation problem, relatively to some targeted microscale constitutive parameters and using a cost function quantifying the discrepancy between the actual macroscale data and predicted data. Two types of measurements can be used: (i) In case of experiments with homogeneous macroscale fields, such as when a tensile test is performed on a standardized specimen, average quantities, such as effective elastic moduli, can be considered (Fedele et al., 2006; Sevenois et al., 2018). For example, Fedele et al. (2006) performed tensile tests on perforated fin-mesh steel sheets, measuring force and average strain, and subsequently identified the elastic-plastic behaviour of the steel through homogenization computations on a representative volume element (RVE). Sevenois et al. (2018) identified carbon fiber properties from composite moduli based on ultrasonic measurements; however, the uncertainties associated with the identified properties remain unclear. Alternatively, (ii) if structural experiments are rather performed, then the produced macroscale data is inherently heterogeneous, to be used as such as Klinge (2012a,b); Schmidt et al. (2015); Burczyński and Kuś (2008). In such cases, displacement fields are typically measured via digital image correlation, and multiscale computational methods, such as FE^2 techniques (Feyel and Chaboche, 2000), can be applied to account for the heterogeneities at both the macro and microscales. While the latter approach is efficient, as it generates a large amount of data from a single test, it is often more complex to implement.

As highlighted by Hartmann and Gilbert (2018), inverse homogenization constitutes an ill-posed problem whose solution existence, uniqueness, and stability are not guaranteed. In this context, significant efforts have been made to analyse structural experiments to extract more information and enhance the likelihood of successful parameter identification. Noticeably, some gradient-based

algorithms for cost functions minimisation, using gradient approximations by finite differences, as well as semi-analytical methods, have been developed (Fish and Ghouali, 2001; M.A. Ghouali et al., 1998). Given the cost of accurate gradient computations, gradient-free algorithms have also been explored (Klinge and Steinmann, 2015; Burczyński and Kuś, 2008), along with techniques related to model-reduction (Oskay and Fish, 2008) or Gaussian processes (Diebels et al., 2018). Using a Monte-Carlo approach, Schmidt et al. (2016) examined the impact of noise in the measured displacement fields on the identified properties, depending on the structural experiment considered. The identification of both linear and nonlinear behaviours have been investigated in the literature.

In the present work, we focus on the quantitative identification of a subset of constitutive parameters in the context of conventional tensile tests, *i.e.* in situations where heterogeneity can be neglected at the macroscale. The unknown microscale parameters are identified from the effective response of the composite and knowledge of the complementary subset of microscale parameters. A solution is obtained by minimizing a cost function which compares measurements of the effective response of the composite to data produced numerically for some candidate parameters, relying on efficient full-field homogenization computations to do so. First and second-order gradient-descent algorithms are considered and compared. To implement the latter, the gradient and Hessian of the cost function must be computed, which requires differentiating the effective response with respect to microscale parameters. To this end and building upon the earlier developments in Bobeth and Diener (1986); Kreher (1990); Suquet and Ponte Castañeda (1993), second-order asymptotic expansions of the effective stress and energy potential are proposed in a general setting, encompassing nonlinear behaviours. The first-order derivatives are shown to be directly computable from the strain fields generated in typical homogenization simulations. A few additional simulations are required to compute the Hessian matrix. These computations are here efficiently performed using the FFT-based homogenization method of Moulinec and Suquet (1994, 1998). These developments are also particularized when the effective response can be expressed in terms of effective parameters, such as in the linear elastic case. In the general nonlinear case, the method is described as a stress or energy-based formulation.

In this article, Section 2 introduces the framework for the direct and inverse homogenization problems. An illustrative analytical example is first studied to highlight some critical issues related to the inverse problem considered, namely the existence and uniqueness of a solution, and its stability. An optimization-based approach is then considered and cost function derivatives are investigated in Section 3 in connection to full-field computations of the arising cell problems posed on the RVE of a given periodic composite. First and second-order derivatives of the effective stress and energy potential are obtained in a general setting, and particularized in the linear elastic case. In addition, it is shown how sensitivity maps can be computed to gain local information within the RVE. A first application example is presented in Section 4, implementing gradient-descent schemes coupled with full-fields simulations to identify isotropic elastic moduli of fibers from the moduli of a composite (matrix+fibres). In order to assess the effects of uncertainties at the optimum found, a linear sensitivity analysis is also performed based on the previous theoretical results. Quantifying these parameter sensitivities makes it possible to assess the propagation of perturbations on each input parameter, and thus to determine the relevant experiments to be carried out to improve the identification procedure. Finally, a second application example is proposed in Section 5 on the identification of the viscoelastic behaviour of a matrix in a glass-fiber composite (with isotropic elastic fibers), also relying on full-field simulations. The previous developments are extended to the viscoelastic setting using the Laplace–Carson transform. In the example considered, the matrix is searched in the form of a generalized Maxwell model, and the moduli of the viscous

branches and the characteristic relaxation times are identified from some complex moduli data for the composite, which can be obtained by dynamical mechanical analysis (DMA) experiments (Audoit et al., 2019). All the examples presented in the present study are based on synthetic data to illustrate the proposed approach while circumventing the so-called inverse crime. All the full-fields computations are performed using FFT-based homogenization techniques.

2. Homogenization problems

This section introduces the framework of the direct and inverse homogenization problems and illustrates their key features on an analytical example.

2.1. Direct homogenization

Consider a periodic composite with representative cell $\Omega \subset \mathbb{R}^d$ and let $\boldsymbol{\eta}$ a vector of constitutive parameters of interest, so that the mechanical behaviour is governed by a local energy density $w(\mathbf{x}, \boldsymbol{\varepsilon}, \boldsymbol{\eta})$, non necessarily quadratic. Given an applied macroscopic strain $\mathbf{E} \in \mathbb{R}_{\text{sym}}^{d \times d}$, the associated mechanical problem is then this of finding the displacement field $\mathbf{u}_\eta$, up to a rigid body motion, that satisfies the following set of equations:

$$\begin{cases} \boldsymbol{\varepsilon}_\eta(\mathbf{x}) = \mathbf{E} + \boldsymbol{\varepsilon}[\mathbf{u}_\eta](\mathbf{x}), & \mathbf{u}_\eta \text{ periodic on } \partial\Omega, \\ \boldsymbol{\sigma}_\eta(\mathbf{x}) = \frac{\partial w}{\partial \boldsymbol{\varepsilon}}(\mathbf{x}, \boldsymbol{\varepsilon}_\eta, \boldsymbol{\eta}), \\ \text{div } \boldsymbol{\sigma}_\eta(\mathbf{x}) = \mathbf{0}, & \boldsymbol{\sigma}_\eta \mathbf{n} \text{ anti-periodic on } \partial\Omega, \end{cases} \quad (1)$$

with $\boldsymbol{\varepsilon}[\cdot]$ denoting the small strain operator, and $\mathbf{n}$ the unit outward normal on $\partial\Omega$.

The introduction of $\boldsymbol{\eta}$ allows to focus on some material parameters of interest. This is a vector that gathers all, or a subset, of the constitutive parameters necessary to characterize the constituents, but it is not a field of parameters. For example, given N homogeneous phases with indicator functions χ_p for $p = 1, \dots, N$, the potential w can be expressed as

$$w(\mathbf{x}, \boldsymbol{\varepsilon}, \boldsymbol{\eta}) = \sum_{p=1}^N w_p(\boldsymbol{\varepsilon}, \boldsymbol{\eta}_p) \chi_p(\mathbf{x}), \quad (2)$$

where $\boldsymbol{\eta}_p$ denotes the collection of material parameters for the phase p , so that one can set $\boldsymbol{\eta} = \{\boldsymbol{\eta}_p, p = 1, \dots, N\}$. The geometry of the microstructure is described through χ_p , so we do not include any geometrical parameters in the vector $\boldsymbol{\eta}$.

From the local fields arising in the microstructure under the loading $\mathbf{E}$, i.e. the solution to (1), then the effective response of the composite can be quantified using the mean stress:

$$\boldsymbol{\Sigma}_\eta = \langle \boldsymbol{\sigma}_\eta \rangle, \quad (3)$$

where $\langle g \rangle = \int_\Omega g(\mathbf{x}) d\mathbf{x} / |\Omega|$. The macroscopic behaviour can also be described using the effective potential given by

$$W_{\text{eff}}(\mathbf{E}, \boldsymbol{\eta}) = \langle w(\mathbf{x}, \boldsymbol{\varepsilon}_\eta, \boldsymbol{\eta}) \rangle, \quad (4)$$

with $\boldsymbol{\varepsilon}_\eta$ solution of (1). According to Hill's lemma, the mean stress satisfies:

$$\boldsymbol{\Sigma}_\eta = \frac{\partial W_{\text{eff}}}{\partial \mathbf{E}}. \quad (5)$$

Remark 1. In general, the effective energy depends only implicitly on $\mathbf{E}$ and $\boldsymbol{\eta}$ via the solution $\boldsymbol{\varepsilon}_{\boldsymbol{\eta}}$ to (1), so there may not exist an explicit form for W_{eff} that can be expressed in terms of a finite number of effective parameters $\boldsymbol{\eta}_{\text{eff}}$ characterizing the composite. For some material behaviours, however, such as in linear elasticity, such a characterization of W_{eff} is possible and, in this case, (4) can be expressed as follows

$$W_{\text{eff}}(\mathbf{E}, \boldsymbol{\eta}) \equiv W_{\text{eff}}(\mathbf{E}, \boldsymbol{\eta}_{\text{eff}}) \quad \text{with} \quad \boldsymbol{\eta}_{\text{eff}} \equiv \boldsymbol{\eta}_{\text{eff}}(\boldsymbol{\eta}).$$

Note that there is no one-to-one correspondence between the entries of $\boldsymbol{\eta}$ and those of $\boldsymbol{\eta}_{\text{eff}}$. The dimension of the latter is indeed smaller.

2.2. Inverse homogenization problem

Let us consider now a composite for which $\boldsymbol{\eta}^*$ denotes a set of target constitutive parameters to be reconstructed. An associated effective response data $\boldsymbol{\Sigma}_{\boldsymbol{\eta}^*}^{\text{d}}$ is assumed to be measured under a given loading $\mathbf{E}$, so that one aims at determining $\boldsymbol{\eta}$ such that $\boldsymbol{\Sigma}_{\boldsymbol{\eta}} = \boldsymbol{\Sigma}_{\boldsymbol{\eta}^*}^{\text{d}}$ by solving (1). In a relaxed form, the reconstruction can rather be achieved by solving

$$\min_{\boldsymbol{\eta}} J(\boldsymbol{\eta}) \tag{6}$$

with

$$J(\boldsymbol{\eta}) = \mathcal{J}(\boldsymbol{\Sigma}_{\boldsymbol{\eta}}) \tag{7}$$

and where $\mathcal{J}(\boldsymbol{\Sigma})$ being a metric returning the distance of a given stress $\boldsymbol{\Sigma}$ to the effective response data $\boldsymbol{\Sigma}_{\boldsymbol{\eta}^*}^{\text{d}}$. A typical choice for $\mathcal{J}(\boldsymbol{\Sigma})$ reads

$$\mathcal{J}(\boldsymbol{\Sigma}) = \frac{1}{2} \|\boldsymbol{\Sigma} - \boldsymbol{\Sigma}_{\boldsymbol{\eta}^*}^{\text{d}}\|^2, \tag{8}$$

using the Frobenius norm. This can be generalized given a set of measured effective responses for various loadings, given that, owing to the adopted notation, the cost function hides the dependence on $\mathbf{E}$, on which $\boldsymbol{\Sigma}_{\boldsymbol{\eta}^*}^{\text{d}}$ and $\boldsymbol{\Sigma}_{\boldsymbol{\eta}}$ both depend on. Similarly, equations (7–8) can be formulated in terms of a measured effective potential $W_{\text{eff}}^{\text{d}}$ when available, instead of an effective response data.

In the cases where a set $\boldsymbol{\eta}_{\text{eff}}(\boldsymbol{\eta})$ of effective parameters can be defined, then, with a slight abuse of notation, the problem (6) can be solved using instead

$$J(\boldsymbol{\eta}) = \mathcal{J}(\boldsymbol{\eta}_{\text{eff}}) \tag{9}$$

in terms of a cost function $\mathcal{J}$ measuring the discrepancy to some effective parameter data $\boldsymbol{\eta}_{\text{eff}}^{\text{d}}(\boldsymbol{\eta}^*) = \boldsymbol{\eta}_{\text{eff}}^{\text{d}}$. For example:

$$\mathcal{J}(\boldsymbol{\eta}_{\text{eff}}) = \frac{1}{2} \|\boldsymbol{\eta}_{\text{eff}} - \boldsymbol{\eta}_{\text{eff}}^{\text{d}}\|^2, \tag{10}$$

in terms of the Euclidean norm.

While the existence of a solution is ensured within the minimisation framework considered, some classical issues relative to the inverse problem considered, in particular the relation between a reconstruction obtained using (7) or (9) and the target $\boldsymbol{\eta}^*$, will be discussed in the next section and illustrated on an analytical example.

2.3. Analytical example

Consider a composite composed of two phases (1 and 2), which we do not describe further, but which is such that its effective bulk and shear moduli are exactly equal to the Hashin-Shtrikman lower bound formulas:

$$\kappa_{\text{eff}} = f_1 \kappa_1 + (1 - f_1) \kappa_2 - \frac{f_1(1 - f_1)(\kappa_1 - \kappa_2)^2}{(1 - f_1)\kappa_1 + f_1\kappa_2 + 4\mu_2/3}, \quad (11)$$

$$\mu_{\text{eff}} = f_1 \mu_1 + (1 - f_1) \mu_2 - \frac{f_1(1 - f_1)(\mu_1 - \mu_2)^2}{(1 - f_1)\mu_1 + f_1\mu_2 + \frac{\mu_2(9\kappa_2 + 8\mu_2)}{6(\kappa_2 + 2\mu_2)}}. \quad (12)$$

where f_1 denotes the volume fraction of the phase 1, and κ_i and μ_i being respectively the bulk and shear moduli of the phase $i = 1, 2$. This choice serves the illustrative purpose of this section, which aims at highlighting key issues in parameter identification. In other words, the Hashin-Shtrikman lower bound formulas are not considered as estimates but as exact values for a composite.

It is now assumed that the given data is $\boldsymbol{\eta}_{\text{eff}}^{\text{d}} = (\kappa_{\text{eff}}^{\text{d}}, \mu_{\text{eff}}^{\text{d}})$ together with $(\kappa_2^{\text{d}}, \mu_1^{\text{d}})$ and f_1^{d} . The remaining constitutive parameters are unknown, so that one sets $\boldsymbol{\eta} = (\kappa_1, \mu_2)$, and sought through a minimisation problem with the following least-squares cost function:

$$J(\boldsymbol{\eta}) = \left(\frac{\kappa_{\text{eff}}(\boldsymbol{\eta}) - \kappa_{\text{eff}}^{\text{d}}}{\kappa_{\text{eff}}^{\text{d}}} \right)^2 + \left(\frac{\mu_{\text{eff}}(\boldsymbol{\eta}) - \mu_{\text{eff}}^{\text{d}}}{\mu_{\text{eff}}^{\text{d}}} \right)^2.$$

For an example application, one sets $(\kappa_2^{\text{d}}, \mu_1^{\text{d}}) = (3, 7)$ GPa, $f_1^{\text{d}} = 0.5$ and a target $\boldsymbol{\eta}^* = (\kappa_1^*, \mu_2^*) = (8, 5)$ GPa to be identified. While physically admissible, the values used here are chosen purely for illustrative purposes, to clearly highlight the challenges inherent to the inverse problem considered. The associated effective behaviour $\boldsymbol{\eta}_{\text{eff}}^{\text{d}} = (\kappa_{\text{eff}}^{\text{d}}, \mu_{\text{eff}}^{\text{d}})$ is computed using (11) and (12). The minimisation problem for the function J above is then solved using iterative methods: either using gradient-descent to generate iterations of the form

$$\boldsymbol{\eta}^{(k+1)} = \boldsymbol{\eta}^{(k)} - \alpha^{(k)} \nabla J(\boldsymbol{\eta}^{(k)}), \quad (13)$$

or Newton's method with:

$$\boldsymbol{\eta}^{(k+1)} = \boldsymbol{\eta}^{(k)} - \alpha^{(k)} [\nabla^2 J(\boldsymbol{\eta}^{(k)})]^{-1} \nabla J(\boldsymbol{\eta}^{(k)}), \quad (14)$$

with the step length α_k being chosen in both cases so as to satisfy the Wolfe conditions, see e.g. [Nocedal and Wright \(2006\)](#). Initialisation guesses are defined using Reuss and Voigt formulas for approximating the macroscopic behaviour, and the iterations are stopped once, at step k , one satisfies $J(\boldsymbol{\eta}^{(k)}) \leq 10^{-6}$.

Figure 1 shows the contour map of J and the iteration paths for the two iterative methods considered. A global minimum is found within the mechanically admissible domain $(\kappa_1, \mu_2 > 0)$, leading to a unique solution. The cost function is smooth, which helps ensure good convergence of the tested algorithms. However, the Hessian $\nabla^2 J$ is not positive definite everywhere, meaning that J may locally be not convex. As a result, the Newton algorithm may sometimes lead to a direction that locally increases the cost function. At such points, the Hessian matrix was regularized by adding a small multiple of the identity to modify the eigenvalues of the Hessian ([Nocedal and Wright, 2006](#)).

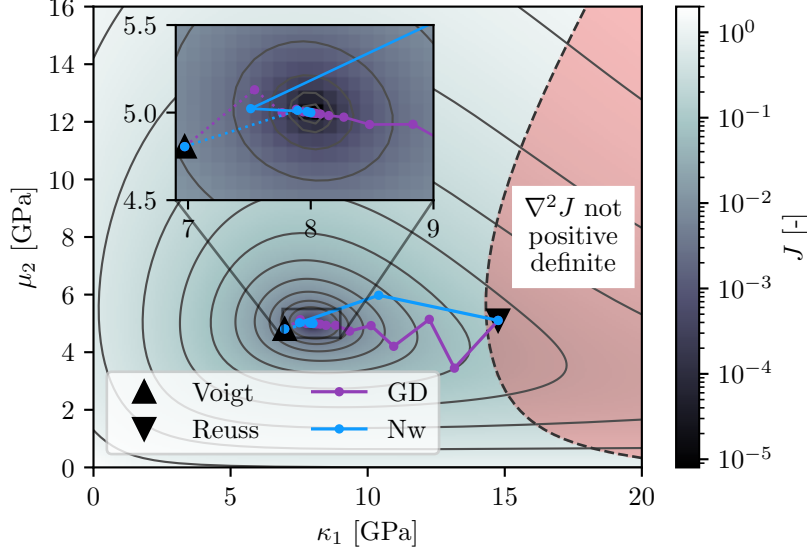


Figure 1: Cost function map with $\eta = (\kappa_1, \mu_2)$. Gradient-descent (GD) and Newton (Nw) algorithms are employed to find a minimum, initial guesses are given by Reuss and Voigt estimates.

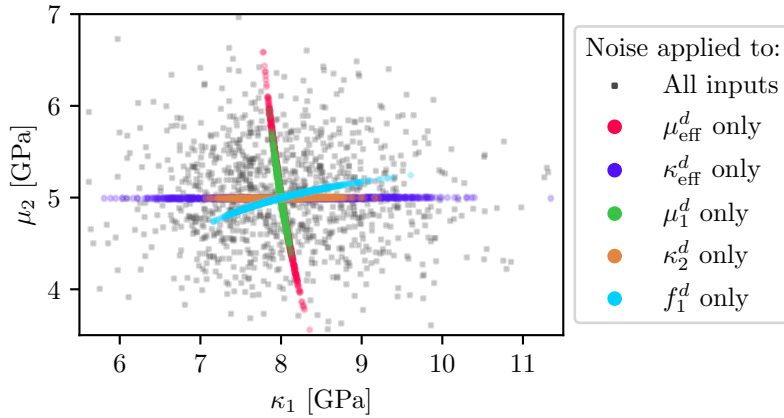


Figure 2: Reconstruction sensitivity with 5% noise. The points correspond to different noisy inputs, either independently or simultaneously.

A numerical sensitivity analysis is also conducted using a Monte Carlo approach, in which the identification as in Figure 1 is performed using 1000 data sets with 5% noise on the inputs, namely the parameters $\kappa_{\text{eff}}^d, \mu_{\text{eff}}^d, \kappa_2^d, \mu_1^d$ and f_1^d . Figure 2 shows the results when noise is applied either individually to each input or to all inputs combined. Since the noise on $\kappa_{\text{eff}}^d, \kappa_2^d$ (resp. $\mu_{\text{eff}}^d, \mu_1^d$) affects almost exclusively the reconstructed parameter κ_1 (resp. μ_2) this problem appears to be relatively bulk/shear decoupled.

Using the same method, Figure 3 (left) shows the map of the cost function J when the data is now $(\kappa_1^d, \kappa_2^d) = (10, 10)$ GPa, $f_1^d = 0.4$ and the target is $(\mu_1^*, \mu_2^*) = (10, 8)$ GPa. In this case, the minimisation schemes considered can lead to multiple solutions as J has locally the shape of a flat valley. Note that the direction of the Newton method (arrows) remains correct even with a non-positive definite Hessian. Finally, a third setup is considered in Figure 3 (right) by prescribing engineers parameters, namely Young's moduli $(E_1^d, E_2^d) = (5, 1)$ GPa and $f_1^d = 0.6$, while the target parameters are now the Poisson's ratios $(\nu_1^*, \nu_2^*) = (-0.1, -0.5)$. The cost function retains the form

of a quadratic sum of relative errors. In this case, solving the minimisation problem is more intricate as the cost function exhibits both a local minimum and a saddle point, see Fig. 3 (right). Once again, the values are not intended to represent a specific material, but rather to illustrate — through plausible scenarios — the potential challenges encountered in inverse homogenization.

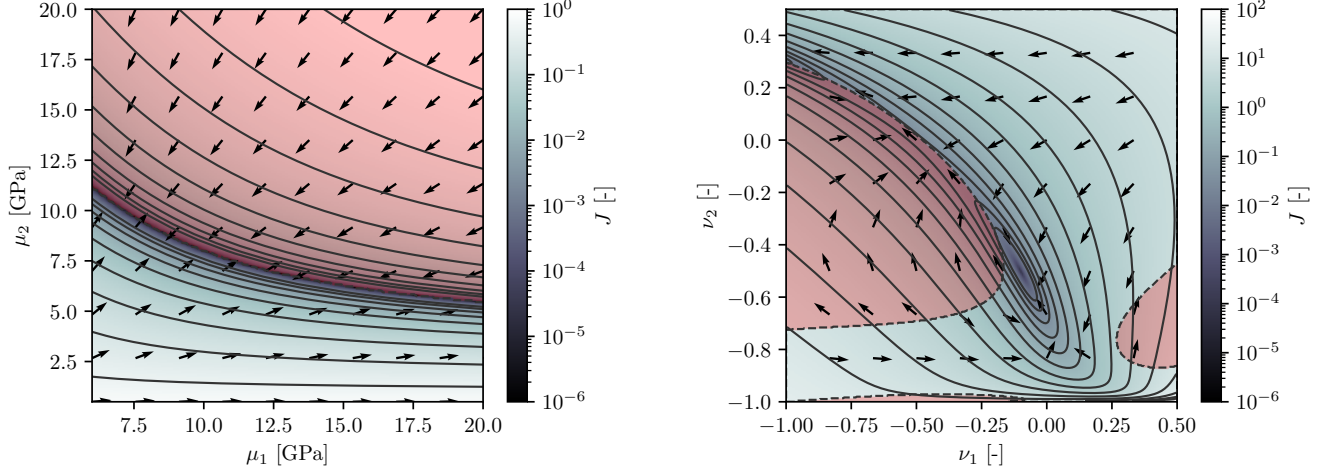


Figure 3: Other examples of the minimisation setup. The arrows represent the vector field of the Newton descent directions $[\nabla^2 J]^{-1} \nabla J$ without modifications, and the red areas are regions where the Hessian matrix is not positive definite as in Fig. 1.

Challenges such as non-uniqueness and convergence to local minima may arise even in relatively simple cases, such as two-phase isotropic composites, see also [Hartmann and Gilbert \(2018\)](#). As illustrated in this analytical example, multiple solutions may coexist depending on the specific choice of unknown parameters, even when only two parameters are to be identified. This highlights the inherent complexity of such an ill-posed problem, for which no general guarantee of uniqueness can be established. Nevertheless, a number of strategies can help detect or mitigate these issues: (i) Evaluating the cost function over a reasonable parameter range can reveal the presence of local minima. (ii) Suitable approximations can serve as effective initial guesses, guiding an optimization scheme towards plausible regions in the parameter space. (iii) Incorporating prior knowledge makes it possible to better restrict the search space. For instance, knowledge of additional elastic moduli can help constrain the solution in the case of anisotropic composites. These issues must be addressed on a case-by-case basis and can be informed by the guidelines outlined above, which we have followed throughout this study. In the following, the effective properties will not be available in closed form, and the reconstruction of constitutive parameters and their sensitivities will be investigated using full-field simulations.

3. Effective response sensitivity

In the previous section, the effective moduli were available in closed-forms, making the calculation of the gradient and Hessian of the cost function analytical. Yet, in general, it is necessary to perform full-field computations of (1) to obtain the effective response, or parameters when the latter can be defined (see Remark 1). Therefore, to minimize the cost function considered using iterative methods such as gradient descent (13) or Newton (14), it is necessary to differentiate it with

respect to the constitutive parameters of interest $\boldsymbol{\eta}$ according to the chain rule. In a stress-based formulation of the cost function (7), the first order derivation lead to:

$$\nabla J(\boldsymbol{\eta}) = \frac{\partial}{\partial \boldsymbol{\eta}} \mathcal{J}(\boldsymbol{\Sigma}(\boldsymbol{\eta})) = \frac{\partial \mathcal{J}}{\partial \boldsymbol{\Sigma}} \frac{\partial \boldsymbol{\Sigma}_{\boldsymbol{\eta}}}{\partial \boldsymbol{\eta}}, \quad (15)$$

and the second order to

$$\nabla^2 J(\boldsymbol{\eta}) = \frac{\partial}{\partial \boldsymbol{\eta}} \left(\frac{\partial \mathcal{J}}{\partial \boldsymbol{\Sigma}} \frac{\partial \boldsymbol{\Sigma}_{\boldsymbol{\eta}}}{\partial \boldsymbol{\eta}} \right) = \frac{\partial \boldsymbol{\Sigma}_{\boldsymbol{\eta}}}{\partial \boldsymbol{\eta}} \frac{\partial^2 \mathcal{J}}{\partial \boldsymbol{\Sigma}^2} \frac{\partial \boldsymbol{\Sigma}_{\boldsymbol{\eta}}}{\partial \boldsymbol{\eta}} + \frac{\partial \mathcal{J}}{\partial \boldsymbol{\Sigma}} \frac{\partial^2 \boldsymbol{\Sigma}_{\boldsymbol{\eta}}}{\partial \boldsymbol{\eta}^2}. \quad (16)$$

Similar derivations can be done in an energy-based formulation with W_{eff} instead of $\boldsymbol{\Sigma}$. Hence, the derivative $\partial \boldsymbol{\Sigma}_{\boldsymbol{\eta}} / \partial \boldsymbol{\eta}$ is key, and relating the latter to the local field fluctuations is the purpose of this section. In this section, we investigate the sensitivity of the effective response of composites to infinitesimal changes in the constitutive parameters $\boldsymbol{\eta}$. This question has been studied, to some extent, in Bobeth and Diener (1986); Kreher (1990); Suquet and Ponte Castañeda (1993).

3.1. Asymptotic expansion of the effective stress

Let us assume that $\boldsymbol{u}_{\boldsymbol{\eta}}$, $\boldsymbol{\sigma}_{\boldsymbol{\eta}}$, and $\boldsymbol{\Sigma}_{\boldsymbol{\eta}}$ are sufficiently smooth and differentiable with respect to the parameter vector $\boldsymbol{\eta}$. We aim at investigating the second-order asymptotic expansion of the effective stress $\boldsymbol{\Sigma}_{\boldsymbol{\eta}}$, which reads

$$\boldsymbol{\Sigma}_{\boldsymbol{\eta} + d\boldsymbol{\eta}} = \boldsymbol{\Sigma}_{\boldsymbol{\eta}} + \frac{\partial \boldsymbol{\Sigma}_{\boldsymbol{\eta}}}{\partial \boldsymbol{\eta}} d\boldsymbol{\eta} + \frac{1}{2} d\boldsymbol{\eta} \frac{\partial^2 \boldsymbol{\Sigma}_{\boldsymbol{\eta}}}{\partial \boldsymbol{\eta}^2} d\boldsymbol{\eta} + o(\|d\boldsymbol{\eta}\|^2) \quad (17)$$

where $\partial \boldsymbol{\Sigma}_{\boldsymbol{\eta}} / \partial \boldsymbol{\eta}$ and $\partial^2 \boldsymbol{\Sigma}_{\boldsymbol{\eta}} / \partial \boldsymbol{\eta}^2$ are the first and second-order Fréchet derivatives of $\boldsymbol{\Sigma}_{\boldsymbol{\eta}}$ viewed as linear and bilinear forms acting on vectors of constitutive parameters.

Remark 2. The leading-order term $\boldsymbol{\Sigma}_{\boldsymbol{\eta}}$ is the mean field associated with the local strain-stress solution $\boldsymbol{\varepsilon}_{\boldsymbol{\eta}}$, $\boldsymbol{\sigma}_{\boldsymbol{\eta}}$ to (1) in the unperturbed configuration, the latter being therefore the zeroth-order terms in an asymptotic expansion of the solution.

3.1.1. First-order derivative

Introducing (3) with the constitutive equation of (1) in (17), and using the chain rule, then the component i of the first-order term is identified as

$$\frac{\partial \boldsymbol{\Sigma}_{\boldsymbol{\eta}}}{\partial \eta_i} = \langle \boldsymbol{C}_t(\boldsymbol{x}, \boldsymbol{\varepsilon}_{\boldsymbol{\eta}}, \boldsymbol{\eta}) \boldsymbol{\varepsilon}'_{\eta_i}(\boldsymbol{x}) + \boldsymbol{\tau}'_{\eta_i}(\boldsymbol{x}, \boldsymbol{\varepsilon}_{\boldsymbol{\eta}}, \boldsymbol{\eta}) \rangle, \quad (18)$$

in terms of the tangent modulus

$$\boldsymbol{C}_t(\boldsymbol{x}, \boldsymbol{\varepsilon}_{\boldsymbol{\eta}}, \boldsymbol{\eta}) = \frac{\partial^2 w}{\partial \boldsymbol{\varepsilon}^2}(\boldsymbol{x}, \boldsymbol{\varepsilon}_{\boldsymbol{\eta}}, \boldsymbol{\eta}), \quad (19)$$

and a stress-like field $\boldsymbol{\tau}'_{\eta_i}$ defined as

$$\boldsymbol{\tau}'_{\eta_i}(\boldsymbol{x}, \boldsymbol{\varepsilon}_{\boldsymbol{\eta}}, \boldsymbol{\eta}) = \frac{\partial \boldsymbol{\sigma}_{\boldsymbol{\eta}}}{\partial \eta_i}(\boldsymbol{x}). \quad (20)$$

In addition, as $d\boldsymbol{\eta}$ does not depend on $\mathbf{x}$, the term $\boldsymbol{\varepsilon}'_{\eta_i}$ in (18) is defined as $\boldsymbol{\varepsilon}'_{\eta_i} = \boldsymbol{\varepsilon}[\mathbf{u}'_{\eta_i}]$ with:

$$\mathbf{u}'_{\eta_i}(\mathbf{x}) = \frac{\partial \mathbf{u}_{\boldsymbol{\eta}}}{\partial \eta_i}(\mathbf{x}) \text{ periodic on } \partial\Omega.$$

By differentiating the equilibrium equation of (1) with respect to $\boldsymbol{\eta}$, then the field $\boldsymbol{\varepsilon}'_{\eta_i}$ can be shown to be the solution of the following cell problem in Ω :

$$\operatorname{div} \left(\mathbf{C}_t(\mathbf{x}, \boldsymbol{\varepsilon}_{\boldsymbol{\eta}}, \boldsymbol{\eta}) \boldsymbol{\varepsilon}'_{\eta_i}(\mathbf{x}) + \boldsymbol{\tau}'_{\eta_i}(\mathbf{x}, \boldsymbol{\varepsilon}_{\boldsymbol{\eta}}, \boldsymbol{\eta}) \right) = \mathbf{0}, \quad (21)$$

with $\langle \boldsymbol{\varepsilon}'_{\eta_i} \rangle = \mathbf{0}$ and where the tangent modulus $\mathbf{C}_t$ is defined in (19) and the prescribed loading $\boldsymbol{\tau}'_{\eta_i}$ in (20) depend on the zeroth-order contribution $\boldsymbol{\varepsilon}_{\boldsymbol{\eta}}$, $\boldsymbol{\sigma}_{\boldsymbol{\eta}}$, see Remark 2.

3.1.2. Second-order derivative

By differentiating (18) then the i, j component of the second-order term in (17) can be identified as

$$\frac{\partial^2 \boldsymbol{\Sigma}_{\boldsymbol{\eta}}}{\partial \eta_i \partial \eta_j} = \left\langle \mathbf{C}_t(\mathbf{x}, \boldsymbol{\varepsilon}_{\boldsymbol{\eta}}, \boldsymbol{\eta}) \boldsymbol{\varepsilon}''_{\eta_i, \eta_j}(\mathbf{x}) + \boldsymbol{\tau}''_{\eta_i, \eta_j}(\mathbf{x}, \boldsymbol{\varepsilon}_{\boldsymbol{\eta}}, \boldsymbol{\varepsilon}'_{\eta_i}, \boldsymbol{\eta}) \right\rangle, \quad (22)$$

where one has defined:

$$\boldsymbol{\tau}''_{\eta_i, \eta_j}(\mathbf{x}, \boldsymbol{\varepsilon}_{\boldsymbol{\eta}}, \boldsymbol{\varepsilon}'_{\eta_i}, \boldsymbol{\eta}) = \left(\frac{\partial \mathbf{C}_t}{\partial \boldsymbol{\varepsilon}} \boldsymbol{\varepsilon}'_{\eta_j} + 2 \frac{\partial \mathbf{C}_t}{\partial \eta_j} \right) \boldsymbol{\varepsilon}'_{\eta_i} + \frac{\partial^2 \boldsymbol{\sigma}_{\boldsymbol{\eta}}}{\partial \eta_i \partial \eta_j}. \quad (23)$$

Moreover, upon differentiating twice the equilibrium equation (1) with respect to $\boldsymbol{\eta}$, then the field $\boldsymbol{\varepsilon}''_{\eta_i, \eta_j}$ in (22), which is defined as $\boldsymbol{\varepsilon}''_{\eta_i, \eta_j} = \boldsymbol{\varepsilon}[\mathbf{u}''_{\eta_i, \eta_j}]$ with $\mathbf{u}''_{\eta_i, \eta_j}(\mathbf{x}) = \partial^2 \mathbf{u}_{\boldsymbol{\eta}} / (\partial \eta_i \partial \eta_j)(\mathbf{x})$ periodic, is found to be solution of the following cell problem in Ω with elasticity defined by the tangent modulus as in (21):

$$\operatorname{div} \left(\mathbf{C}_t(\mathbf{x}, \boldsymbol{\varepsilon}_{\boldsymbol{\eta}}, \boldsymbol{\eta}) \boldsymbol{\varepsilon}''_{\eta_i, \eta_j}(\mathbf{x}) + \boldsymbol{\tau}''_{\eta_i, \eta_j}(\mathbf{x}, \boldsymbol{\varepsilon}_{\boldsymbol{\eta}}, \boldsymbol{\varepsilon}'_{\eta_i}, \boldsymbol{\eta}) \right) = \mathbf{0}, \quad (24)$$

with $\langle \boldsymbol{\varepsilon}''_{\eta_i, \eta_j} \rangle = \mathbf{0}$, and the prescribed loading $\boldsymbol{\tau}''_{\eta_i, \eta_j}$ of (23).

Remark 3. As in (18) where the first-order derivative requires the additional solutions $\boldsymbol{\varepsilon}'_{\eta_i}$ to be computed using $\boldsymbol{\varepsilon}_{\boldsymbol{\eta}}$ through (21), the second-order derivative (22) necessitates the solutions $\boldsymbol{\varepsilon}''_{\eta_i, \eta_j}$ to (24) for which $\boldsymbol{\varepsilon}'_{\eta_i}$ are in turn needed.

Finally, the gradient and Hessian matrix of J are given by using (18) and (22) in (16).

3.2. Extension to the effective potential

Given the results (18) and (22) regarding the effective stress derivatives, their counterparts related to the effective potential can be obtained using Hill's lemma and the cell problems introduced previously. The results below are connected to those in Suquet and Ponte Castañeda (1993), although the latter were formulated in a slightly more restrictive setting. As a preliminary remark, note first that since the macroscopic stress derives from the effective potential, see (5), then for all $j \geq 0$:

$$\frac{\partial^j W_{\text{eff}}}{\partial \eta_i^j} = \int \frac{\partial^j \boldsymbol{\Sigma}_{\boldsymbol{\eta}}}{\partial \eta_i^j} d\mathbf{E} = \frac{\partial^j}{\partial \eta_i^j} \langle w(\mathbf{x}, \boldsymbol{\varepsilon}_{\boldsymbol{\eta}}, \boldsymbol{\eta}) \rangle.$$

3.2.1. First-order derivative

The identity above with $n = 1$ leads to for the component i

$$\frac{\partial W_{\text{eff}}}{\partial \eta_i} = \left\langle \frac{\partial w}{\partial \boldsymbol{\varepsilon}} \cdot \boldsymbol{\varepsilon}'_{\eta_i} + \frac{\partial w}{\partial \eta_i} \right\rangle \quad (25)$$

where $\cdot$ is a scalar product.

As $\boldsymbol{\sigma}_\eta = \partial w / \partial \boldsymbol{\varepsilon}$ is statically admissible, multiplying the equilibrium equation of (1) by the periodic field $\mathbf{u}'_{\eta_i}$ and integrating by parts give:

$$\langle (\text{div } \boldsymbol{\sigma}_\eta) \mathbf{u}'_{\eta_i} \rangle = - \left\langle \frac{\partial w}{\partial \boldsymbol{\varepsilon}} \cdot \boldsymbol{\varepsilon}'_{\eta_i} \right\rangle = 0.$$

Therefore, using (25), we finally obtain:

$$\frac{\partial W_{\text{eff}}}{\partial \eta_i}(\mathbf{E}, \boldsymbol{\eta}) = \left\langle \frac{\partial w}{\partial \eta_i}(\mathbf{x}, \boldsymbol{\varepsilon}_\eta, \boldsymbol{\eta}) \right\rangle. \quad (26)$$

3.2.2. Second-order derivative

Differentiating the identity just obtained and using the definition (20) lead to

$$\frac{\partial^2 W_{\text{eff}}}{\partial \eta_i \partial \eta_j} = \left\langle \frac{\partial^2 w}{\partial \boldsymbol{\varepsilon} \partial \eta_i} \cdot \boldsymbol{\varepsilon}'_{\eta_j} + \frac{\partial^2 w}{\partial \eta_i \partial \eta_j} \right\rangle = \left\langle \boldsymbol{\tau}'_{\eta_i} \cdot \boldsymbol{\varepsilon}'_{\eta_j} + \frac{\partial^2 w}{\partial \eta_i \partial \eta_j} \right\rangle. \quad (27)$$

Now, as $\boldsymbol{\varepsilon}'_{\eta_i}$ is solution to the cell problem (21), multiplying the latter by $\mathbf{u}'_{\eta_j}$ and integrating by parts give

$$\left\langle \boldsymbol{\tau}'_{\eta_i} \cdot \boldsymbol{\varepsilon}'_{\eta_j} \right\rangle = - \left\langle \boldsymbol{\varepsilon}'_{\eta_i} \cdot \mathbf{C}_t \boldsymbol{\varepsilon}'_{\eta_j} \right\rangle.$$

Replacing this term in (27) finally yields

$$\frac{\partial^2 W_{\text{eff}}}{\partial \eta_i \partial \eta_j}(\mathbf{E}, \boldsymbol{\eta}) = \left\langle \frac{\partial^2 w}{\partial \eta_i \partial \eta_j}(\mathbf{x}, \boldsymbol{\varepsilon}_\eta, \boldsymbol{\eta}) - \boldsymbol{\varepsilon}'_{\eta_i}(\mathbf{x}) \cdot \mathbf{C}_t(\mathbf{x}, \boldsymbol{\varepsilon}_\eta, \boldsymbol{\eta}) \boldsymbol{\varepsilon}'_{\eta_j}(\mathbf{x}) \right\rangle. \quad (28)$$

with $\boldsymbol{\varepsilon}'_{\eta_i}$ and $\boldsymbol{\varepsilon}'_{\eta_j}$ found by solving (21).

Remark 4. Considering an optimization problem based on the effective energy (or parameters) instead of the macroscopic stress offers therefore a significant advantage because of the fields required to compute the derivatives of the associated cost function. In the case of a formulation based on the effective energy, no additional solution to $\boldsymbol{\varepsilon}_\eta$ is needed for the first-order derivative (26), while the second-order one (28) only requires knowledge of the $\boldsymbol{\varepsilon}'_{\eta_i}$, to be compared with $\boldsymbol{\varepsilon}'_{\eta_i}$ and the second-order term $\boldsymbol{\varepsilon}''_{\eta_i, \eta_j}$ being involved in (18) and (22), respectively.

3.2.3. Linear elastic and isotropic case

Here, we particularize the results of the previous subsections in $\mathbb{R}^3$ and for a piecewise homogeneous composite made of N phases Ω_p , see (2), which are linear elastic and isotropic so that the energy density w_p is quadratic and writes as

$$w_p(\boldsymbol{\varepsilon}, \boldsymbol{\eta}_p) = \frac{\kappa_p}{2} \text{tr}(\boldsymbol{\varepsilon})^2 + \mu_p \text{dev}(\boldsymbol{\varepsilon}) \cdot \text{dev}(\boldsymbol{\varepsilon}),$$

where κ_p, μ_p are the bulk and shear moduli, respectively, of each phase with indicator function χ_p , and with $\text{dev}(\boldsymbol{\varepsilon}) = \boldsymbol{\varepsilon} - \frac{1}{3} \text{tr}(\boldsymbol{\varepsilon}) \mathbf{I}$ denoting the deviatoric strain field. In such a case, the constitutive parameter vector $\boldsymbol{\eta}$ is defined as

$$\boldsymbol{\eta} = (\kappa_1, \mu_1, \dots, \kappa_N, \mu_N). \quad (29)$$

In such a case, using (26), the first-order derivatives with respect to the moduli of each phase p simplify to

$$\begin{cases} \frac{\partial W_{\text{eff}}}{\partial \kappa_p}(\mathbf{E}, \boldsymbol{\eta}) = \frac{f_p}{2} \left\langle \text{tr}(\boldsymbol{\varepsilon}_{\boldsymbol{\eta}}(\mathbf{x}))^2 \right\rangle_{(p)}, \\ \frac{\partial W_{\text{eff}}}{\partial \mu_p}(\mathbf{E}, \boldsymbol{\eta}) = f_p \left\langle \text{dev}(\boldsymbol{\varepsilon}_{\boldsymbol{\eta}}(\mathbf{x})) \cdot \text{dev}(\boldsymbol{\varepsilon}_{\boldsymbol{\eta}}(\mathbf{x})) \right\rangle_{(p)} \end{cases} \quad (30)$$

with the volume fraction $f_p = |\Omega_p|/|\Omega|$ of the phase p and the associated local averaging operator $\langle g \rangle_{(p)} = \int_{\Omega_p} g(\mathbf{x}) d\mathbf{x} / |\Omega_p|$. In (30), the field $\boldsymbol{\varepsilon}_{\boldsymbol{\eta}}$ is the total strain $\boldsymbol{\varepsilon}_{\boldsymbol{\eta}} = \mathbf{E} + \boldsymbol{\varepsilon}[\mathbf{u}_{\boldsymbol{\eta}}]$ with $\mathbf{u}_{\boldsymbol{\eta}}$ solution of the unperturbed problem (1), i.e. such that:

$$\text{div}(\mathcal{C}(\mathbf{x}, \boldsymbol{\eta}) \boldsymbol{\varepsilon}[\mathbf{u}_{\boldsymbol{\eta}}](\mathbf{x}) + \boldsymbol{\tau}(\mathbf{x}, \mathbf{E}, \boldsymbol{\eta})) = \mathbf{0}, \quad (31)$$

with given polarization stress

$$\boldsymbol{\tau}(\mathbf{x}, \mathbf{E}, \boldsymbol{\eta}) = \mathcal{C}(\mathbf{x}, \boldsymbol{\eta}) \mathbf{E},$$

and where

$$\mathcal{C}(\mathbf{x}, \boldsymbol{\eta}) = \sum_{p=1}^N (3\kappa_p \mathbf{J} + 2\mu_p \mathbf{K}) \chi_p(\mathbf{x})$$

in terms of the spherical and deviatoric fourth-order projection tensors $\mathbf{J}$ and $\mathbf{K}$, respectively.

The second-order derivatives can be obtained using (28) upon noting that $\partial^2 w / (\partial \eta_i \partial \eta_j) = \mathbf{0}$ in the linear case considered, so that

$$\frac{\partial^2 W_{\text{eff}}}{\partial \eta_i \partial \eta_j}(\mathbf{E}, \boldsymbol{\eta}) = - \left\langle \boldsymbol{\varepsilon}'_{\eta_i}(\mathbf{x}) \cdot \mathcal{C}(\mathbf{x}, \boldsymbol{\eta}) \boldsymbol{\varepsilon}'_{\eta_j}(\mathbf{x}) \right\rangle, \quad (32)$$

since the tangent modulus $\mathbf{C}_t$ in (19) reduces to

$$\mathbf{C}_t(\mathbf{x}, \boldsymbol{\varepsilon}_{\boldsymbol{\eta}}, \boldsymbol{\eta}) = \mathcal{C}(\mathbf{x}, \boldsymbol{\eta}).$$

In addition, the fields $\boldsymbol{\varepsilon}'_{\eta_i}$ in (32) are defined by the cell problem (21), i.e. the components $\boldsymbol{\varepsilon}'_{\kappa_p}$ and $\boldsymbol{\varepsilon}'_{\mu_p}$ for all $p = 1, \dots, N$ derive from periodic displacement fields and are the solutions to

$$\begin{cases} \text{div}(\mathcal{C}(\mathbf{x}, \boldsymbol{\eta}) \boldsymbol{\varepsilon}'_{\kappa_p}(\mathbf{x}) + \boldsymbol{\tau}'_{\kappa_p}(\mathbf{x}, \boldsymbol{\varepsilon}_{\boldsymbol{\eta}})) = \mathbf{0} \\ \boldsymbol{\tau}'_{\kappa_p}(\mathbf{x}, \boldsymbol{\varepsilon}_{\boldsymbol{\eta}}) = \text{tr}(\boldsymbol{\varepsilon}_{\boldsymbol{\eta}}(\mathbf{x})) \chi_p(\mathbf{x}) \mathbf{I}, \end{cases}$$

and

$$\begin{cases} \text{div}(\mathcal{C}(\mathbf{x}, \boldsymbol{\eta}) \boldsymbol{\varepsilon}'_{\mu_p}(\mathbf{x}) + \boldsymbol{\tau}'_{\mu_p}(\mathbf{x}, \boldsymbol{\varepsilon}_{\boldsymbol{\eta}})) = \mathbf{0} \\ \boldsymbol{\tau}'_{\mu_p}(\mathbf{x}, \boldsymbol{\varepsilon}_{\boldsymbol{\eta}}) = 2 \text{dev}(\boldsymbol{\varepsilon}_{\boldsymbol{\eta}}(\mathbf{x})) \chi_p(\mathbf{x}). \end{cases}$$

3.3. Derivatives of effective elasticity parameters

When elastic phases are considered then effective parameters $\boldsymbol{\eta}_{\text{eff}}$ can be defined, see Remark 1, and an associated minimisation strategy can be adopted, for example using (10). The vector $\boldsymbol{\eta}_{\text{eff}}$ typically gathers constitutive moduli which can be expressed as functions of the entry $c_{ijkl,\text{eff}}$ of the effective stiffness tensor $\mathbf{C}_{\text{eff}}$. The computation of the derivatives of the cost function $\mathcal{J}(\boldsymbol{\eta}_{\text{eff}}(\boldsymbol{\eta}))$ is then done by chain-rule derivations

$$\frac{\partial J}{\partial \boldsymbol{\eta}} = \frac{\partial \mathcal{J}}{\partial \boldsymbol{\eta}_{\text{eff}}} \frac{\partial \boldsymbol{\eta}_{\text{eff}}}{\partial c_{ijkl,\text{eff}}} \frac{\partial c_{ijkl,\text{eff}}}{\partial \boldsymbol{\eta}}$$

and similarly for the second-order derivative. While the computation of the two first right-hand side terms is straightforward, the computation of $\partial c_{ijkl,\text{eff}}/\partial \boldsymbol{\eta}$ can be done using the energy-based derivatives (26) and (28) for some well-chosen loadings. For example, using $\mathbf{E}$ such as:

$$\mathbf{E} = \varepsilon_0(\mathbf{e}_i \otimes \mathbf{e}_j)_{\text{sym}}$$

then the effective potential is $W_{\text{eff}} = c_{ijij,\text{eff}}\varepsilon_0^2/2$, which leads to

$$\frac{\partial c_{ijij,\text{eff}}}{\partial \boldsymbol{\eta}} = \frac{2}{\varepsilon_0^2} \frac{\partial W_{\text{eff}}}{\partial \boldsymbol{\eta}}(\mathbf{E}, \boldsymbol{\eta}).$$

The derivatives of the remaining 15 independent coefficients (for an elasticity tensor exhibiting both major and minor symmetries) can be derived through linear combinations. For example, the derivative of the coefficient $c_{ijkl,\text{eff}}$ can be obtained by combining the two loadings:

$$\mathbf{E}_1 = \varepsilon_0(\mathbf{e}_i \otimes \mathbf{e}_j)_{\text{sym}} \quad \text{and} \quad \mathbf{E}_2 = \varepsilon_0[(\mathbf{e}_i \otimes \mathbf{e}_j) + (\mathbf{e}_k \otimes \mathbf{e}_\ell)]_{\text{sym}}.$$

This procedure is applied in the same way to determine the second-order derivatives of the elasticity tensor entries from (32).

3.4. Local fluctuations and sensitivity maps

With $\boldsymbol{\eta}$ seen as a collection of constitutive parameters, let us focus on the fluctuation of a given parameter $m(\mathbf{z}) \subset \boldsymbol{\eta}$ which we assume to be uniform in a ball $B_a(\mathbf{z})$ of radius a around a point $\mathbf{z} \in \Omega$, i.e. we consider the material perturbation given by:

$$m(\mathbf{z}) \leftarrow m(\mathbf{z}) + \text{d}m \quad \text{in} \quad B_a(\mathbf{z}).$$

In such a case, once (1) has been solved then the first-order derivative (26) with respect to $m(\mathbf{z})$ can be approximated as

$$\frac{\partial W_{\text{eff}}}{\partial m(\mathbf{z})}(\mathbf{E}, \boldsymbol{\eta}) \underset{a \rightarrow 0}{\approx} f_a \frac{\partial w}{\partial m(\mathbf{z})}(\mathbf{z}, \boldsymbol{\varepsilon}_\eta, \boldsymbol{\eta}), \quad (33)$$

where $f_a \propto a^d/|\Omega|$ stands for the volume fraction of $B_a(\mathbf{z}) \subset \mathbb{R}^d$ as the energy density w , which depends only on the local constitutive properties, is assumed to be smooth at $\mathbf{z}$ and thus uniform in $B_a(\mathbf{z})$ when $a \rightarrow 0$. The equation (33) then allows us to define a sensitivity maps $S_m(\mathbf{z})$ as

$$S_m(\mathbf{z}) : \mathbf{z} \mapsto \frac{\partial w}{\partial m(\mathbf{z})}(\mathbf{z}, \boldsymbol{\varepsilon}_\eta, \boldsymbol{\eta}), \quad (34)$$

which is a field defined in the representative cell Ω that quantifies the sensitivity of the effective potential W_{eff} to a local fluctuation of the parameter m at the point $\mathbf{z}$.

4. Identification of elastic phases

This section uses inverse homogenization and the tools introduced in the previous section to identify elastic phases in a composite. The method is illustrated in the case of a fibre-reinforced plastic composite. While the behaviours of the composite and of the matrix are assumed to be known, the objective is to identify the properties of the fibres.

4.1. Example of a fibre-reinforced composite

4.1.1. Problem setting

In this example, we consider a two-phase composite made of fibres randomly stacked and embedded in a matrix phase, as in Figure 4a. Both constituents are isotropic elastic and the reference

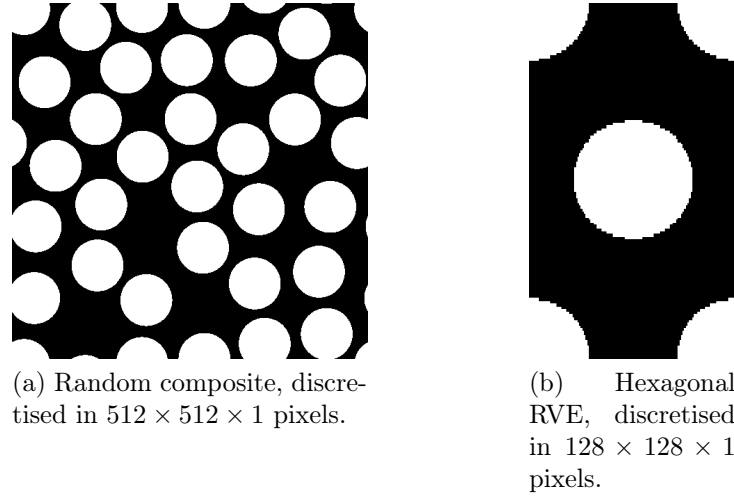


Figure 4: Composite configurations considered in the numerical examples.

values for their parameters (Young’s modulus and Poisson’s ratio) are given in Table 1. The chosen values are representative of typical glass fiber and polymer matrix within glass-fibre composites (Soden et al., 1998). The fibre fraction is set to 50%. In this setting, we aim at identifying the bulk and shear moduli of the fibres, so that one sets $\boldsymbol{\eta} = (\kappa_f, \mu_f)$. The targeted version $\boldsymbol{\eta}^* = (38.89, 29.17)$ GPa of the latter is computed from Table 1.

Phase	E^* [GPa]	ν^* [-]	μ^* [GPa]	κ^* [GPa]
Matrix	5.0	0.4	1.79	8.33
Fibre	70.0	0.2	29.17	38.89

Table 1: Reference and targeted parameter values.

The two matrix parameters are assumed to be known, which we denote as $(\kappa_m^d, \mu_m^d) = (8.33, 1.79)$ GPa, as well as the fibre fraction $f^d = 0.5$. Due to the geometry of the microstructure, the effective material is supposed transverse isotropic, entirely described by five parameters. Among these, it is first assumed that the only available data is the longitudinal Young’s and shear moduli, which we denote as $E_{\ell, \text{eff}}^d, \mu_{\ell, \text{eff}}^d$, respectively. This choice is made as these moduli require minimal experimental setup to be measured in practice. The cost function considered is defined as:

$$J(\boldsymbol{\eta}) = \left(\frac{E_{\ell, \text{eff}}(\boldsymbol{\eta}) - E_{\ell, \text{eff}}^d}{E_{\ell, \text{eff}}^d} \right)^2 + \left(\frac{\mu_{\ell, \text{eff}}(\boldsymbol{\eta}) - \mu_{\ell, \text{eff}}^d}{\mu_{\ell, \text{eff}}^d} \right)^2. \quad (35)$$

4.1.2. Computational aspects

The effective behaviour of the composite material is computed using 3D full-field simulations. We employ FFT-based homogenization techniques, which are particularly efficient compared to traditional FE methods. For the computations, we use the scheme proposed by [Moulinec and Suquet \(1994\)](#) along with the stopping criteria outlined by [Bellis and Suquet \(2019\)](#) (set at 10^{-6}).

The RVE consists of 30 fibers that are randomly distributed and discretized into a grid of $512 \times 512 \times 1$ pixels, resulting in 3.1 million degrees of freedom (see Figure 4a). To compute the effective stiffness tensor, six successive loadings are applied, and the effective energy is calculated using the following equation:

$$W_{\text{eff}} = \frac{1}{2} \boldsymbol{\Sigma} \cdot \mathbf{E} = \frac{1}{2} \mathbf{E} \cdot \mathbf{C}_{\text{eff}} \mathbf{E}.$$

Alternatively, the effective stiffness tensor can be calculated by the mean of the stress, with sometimes fewer loadings, see ([Kanit et al., 2003](#)). However, the energy-based formulation converges with fewer FFT iterations than the stress-based one ([Bellis et al., 2020](#)). The identification of the fiber parameters is performed using the gradient-based schemes discussed in the previous sections.

Preliminary to the identification process, synthetic data for the moduli ($E_{\ell, \text{eff}}^{\text{d}}, \mu_{\ell, \text{eff}}^{\text{d}}$) are computed using the reference parameters of the fiber. To avoid the so-called "inverse crime," these moduli are calculated using a different homogenization scheme, namely this of [Eyre and Milton \(1999\)](#), than the one used for the identification. Moreover, the RVE employed is the one Figure 4a with a 10° tilted angle to change the local discretization.

The algorithms tested to minimize the cost function are:

- Newton: the gradient and the Hessian matrix of the cost function, ∇J and $\nabla^2 J$, are respectively computed with (26), (28) and (15). At each iteration, six loadings are performed to compute the effective stiffness by the mean energy, using the cell problem (31) at the zeroth-order. While the gradient of the cost function is computed from the previous solution fields, the Hessian matrix requires solving the cell problem (21) for $6 \times 2 = 12$ loadings to compute $\mathbf{u}'_{\eta}$ for both the unknowns κ_f and μ_f . In total, 18 loadings of elastic cell problems are computed at each iteration of the scheme.
- Quasi-Newton: the difference with the Newton algorithm stands with the computation of the Hessian matrix of the cost function $\nabla^2 J$. Instead of solving the cell problem (21), the second-order derivatives are approximated by finite differences of the gradient. In total, the cell problem (31) is solved for 18 loadings.
- BFGS: at the first iteration, the approximation of the Hessian matrix is set to the identity. For the next iterations, only the function's gradient is needed, so only a total of 6 loadings are computed per iteration.

At each iteration, the step length α_k is determined using a line search method that meets the Wolfe conditions, as described by [Nocedal and Wright \(2006\)](#). For efficiency, the computations for the step length search are conducted with a low-fidelity stopping criterion set at 5×10^{-5} , in contrast to the standard 10^{-6} . To ensure the elasticity tensor of the identified fibres remains positive definite, the moduli κ_f and μ_f are constrained to be strictly positive by expressed as exponentials. Additionally, within the (quasi-)Newton algorithm, the Hessian matrix undergoes regularization to guarantee a favourable search direction, even when negative eigenvalues are present. This is

achieved by adding a multiple of the identity, as outlined by Nocedal and Wright (2006). The update for the next iteration is given by:

$$\boldsymbol{\eta}^{(k+1)} = \boldsymbol{\eta}^{(k)} - \alpha^{(k)} [\beta \mathbf{I} + \nabla^2 J(\boldsymbol{\eta}^{(k)})]^{-1} \nabla J(\boldsymbol{\eta}^{(k)}),$$

where $\beta = \max(0, \delta - \lambda_{\min})$, with $\lambda_{\min}$ representing the minimal eigenvalue of the Hessian matrix and δ a parameter arbitrarily set at 10^{-5} .

Remark 5. *The iterative gradient-based identification methods considered require solving repeatedly the periodic cell problems (31), (21) and (24), which all retain the same form. A fast numerical platform is therefore needed to do so and, as already discussed in (Cornaggia and Bellis, 2020), the FFT-based spectral methods considered here provide an effective solution.*

4.2. Identification results

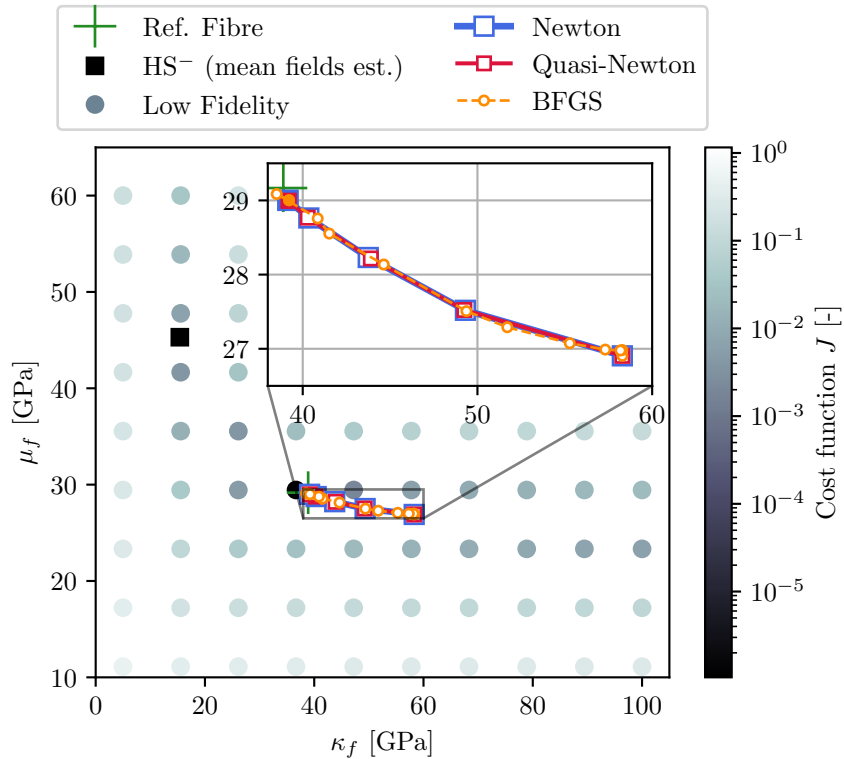


Figure 5: Identification of the fibre properties: prior estimate and iterative identification.

To choose an initialization guess, we can consider a first guess for the targeted constitutive properties using a preliminary inversion from a mean-field approximation of the composite behaviour, either analytically or numerically as in Section 2.3. For example, using the Hashin-Shtrikman lower bound (HS⁻) for a composite with cylindrical inclusions, we obtain a first approximation of the fibre properties, see Figure 5. The quality of this approximated guess is rather poor. One may attempt with a more accurate estimate of the composite properties, like the generalized self-consistent estimate, but we instead perform a low-fidelity mapping of the cost function, Fig. 5. In the context considered here, this is achieved by performing FFT-based full-field computations with a low-precision convergence criterion. One could also consider a coarser discretization of the RVE, in particular in the context of the finite element method.

Figure 5 illustrates the paths and the identification results using the tested algorithms. For a user-chosen value of the cost function of 10^{-6} , the Newton, quasi-Newton and BFGS converge in 4, 4 and 12 iterations, respectively. Considering that BFGS requires three times less simulations per step, it is faster to compute. No convergence issues were encountered in the performed computations. Other initialization points within the range of Figure 5 were tested and consistently produced similar results. For the worst initial guess, 20 iterations using the BFGS algorithm were required. The residual gaps of about 1% between the reference and the algorithm results are due to the stopping criteria of the iterative identification and the manner in which the reference data has been computed to avoid the inverse crime. The stopping criterion value has a relatively minor impact on the results, as evidenced by the observation that modifying it to 10^{-9} yields a change of only 0.1% in the computed output.

4.3. Sensitivity analysis

4.3.1. Sensitivity maps

As discussed in Section 3.4, sensitivity maps can be generated directly from the displacement fields solution of the problem (1) with (34). Figure 6 displays such maps for the transverse isotropic effective parameters $E_{\ell,\text{eff}}$, $E_{t,\text{eff}}$, and $\mu_{\ell,\text{eff}}$ w.r.t. to the local shear, bulk and Young moduli of both the fibres and the matrix.

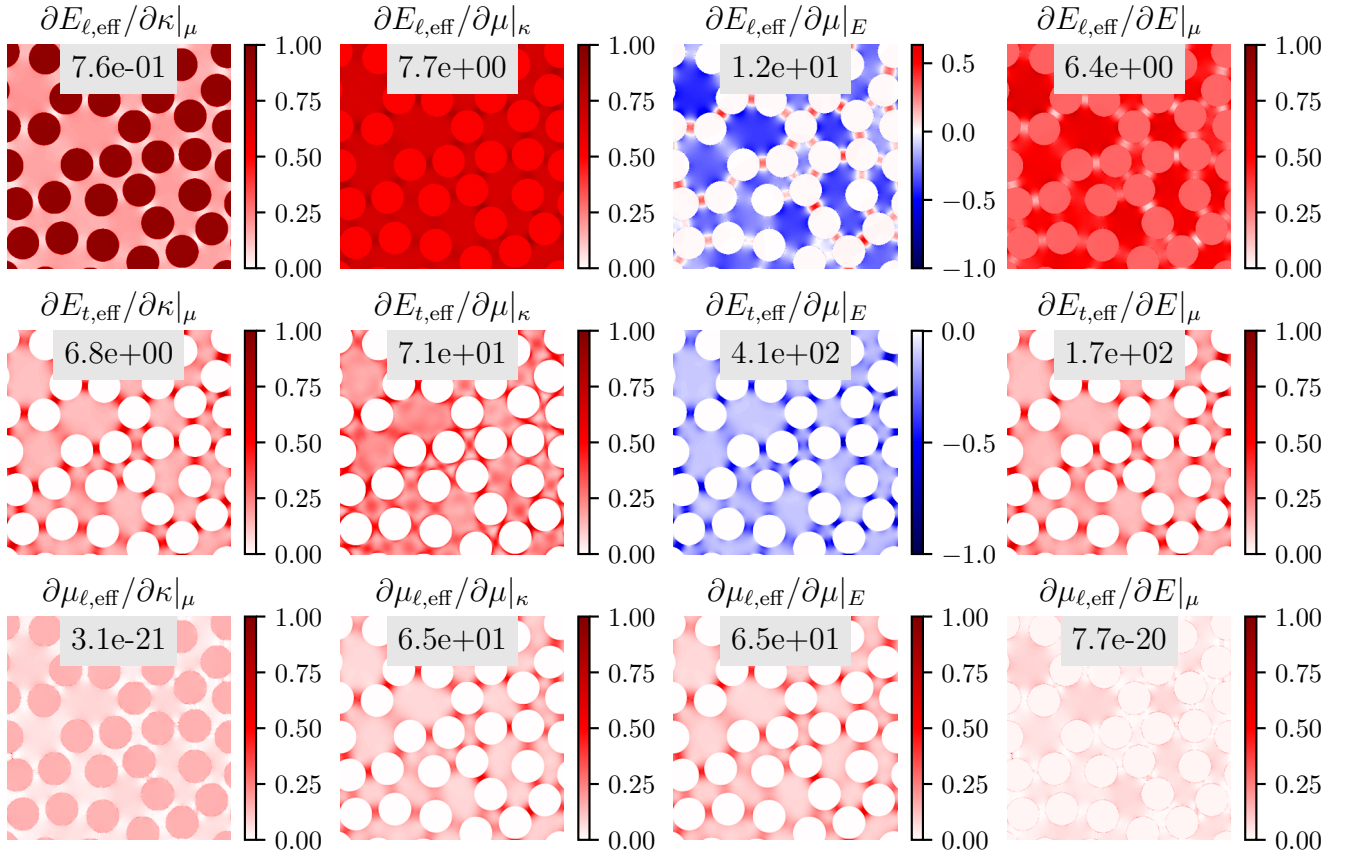


Figure 6: Normalized sensitivity maps of three effective moduli $E_{\ell,\text{eff}}$, $E_{t,\text{eff}}$, $\mu_{\ell,\text{eff}}$, relatively to the local shear $\mu(\mathbf{x})$, bulk $\kappa(\mathbf{x})$, and Young $E(\mathbf{x})$ moduli. The normalization factor is reported in grey box. The derivative $\partial X/\partial x|_y$ denote the derivative of X w.r.t. x with y kept constant.

Two cases are distinguished whether the bulk or the Young modulus is considered constant for

the partial derivatives. Both the average and local data from those may be extract in different context for several applications:

- Dependence of micro to macro scale parameters: Understanding the impact of phase parameters on macroscale factors can guide the selection of which parameters to optimize for enhancing specific effective behaviours. It is important to note that increasing a given phase modulus does not consistently result in a higher effective stiffness, as this depends on the elastic parameters in question. For instance, when the matrix modulus μ increases with a constant E , the effective tensile modulus $E_{t,\text{eff}}$ decreases. Furthermore, local variations can lead to either an increase or decrease in effective stiffness based on their location. Specifically, the composite modulus $E_{\ell,\text{eff}}$ is enhanced when the matrix surrounding closed fibres increases, while it may decrease in other areas. Considering the alternative parameters (κ, μ) , varying conclusions regarding the assessed composite moduli can be made. Finally, the dependence of parameters is key for experimental testing towards inverse homogenization. Some effective moduli do not rely on local parameters; for example, the shear modulus $\mu_{\ell,\text{eff}}$ is determined exclusively by the shear moduli of the matrix because it is obtained by anti-planar loading that generates only local shear strain. The key takeaway is that different scenarios can significantly influence sensitivities, making it challenging to anticipate the expected outcomes based on the selected microstructure and phase contrast. In the present example, the cost function involving $E_{\ell,\text{eff}}$ and $\mu_{\ell,\text{eff}}$ is justified for κ^f and μ^f respectively. In the case where the matrix is to be identified rather than the fibers, $E_{t,\text{eff}}$ would be a more relevant choice than $E_{\ell,\text{eff}}$.
- Random RVE size assessment: These maps offer valuable insights into the factors influencing the size of the representative volume element (RVE) through the identification of highly sensitive areas. Because these areas drive the effective behaviour of the material, their representation within the RVE must be sufficient to dictate the overall size for random microstructures. In the context of unidirectional (UD) composites, the RVE issue has been extensively examined, often with a focus on stress maps under specific loading conditions (Huang et al., 2008; Younes et al., 2012; Merlette and Diani, 2025). However, in this case, the relationship between the phases and effective parameters is clearly articulated. The effective response is significantly influenced by the matrix surrounding closely spaced fibers. Consequently, the RVE size is directly determined by the characteristics of these regions, including their number, orientation, and spatial extent. Notably, the minimum distance between fibers stands out as a critical factor affecting the RVE size; specifically, the closer the fibers are within the domain, the larger the RVE must be to accurately represent configurations in which the fibers are in close proximity to each other (due to *cusp* singularities). To better quantify the effect on the RVE size, a dedicated method like the integral range method (Kanit et al., 2003) remains required.
- Local microstructure and phase sensitivities: The maps offer insights into local sensitivities within the microstructure, enabling the enhancement of specific effective properties by adjusting parameters at a local level. For instance, one might examine a local property in $\boldsymbol{\eta}(\boldsymbol{x})$ (such as shear modulus or phase index) represented on a discretized grid. Lastly, one may investigate these maps to assess the stability of a microstructure design *w.r.t.* geometrical uncertainties/defects.

4.3.2. Approximations of uncertainties

When Hessian-based algorithms are used, the eigenvalues and eigenvectors of second-order derivatives $\nabla^2 J$ can be computed to estimate the direction of major sensitivity of the identified parameters. In the example considered where $\boldsymbol{\eta} = (\kappa_f, \mu_f)$ is identified, the eigenvalues and eigenvectors of the Hessian matrix are at the optimal point :

$$\begin{cases} \lambda_1 = 1.9 \times 10^{-6} & \boldsymbol{\eta}_{\lambda_1} = (0.99, 0.17), \\ \lambda_2 = 1.4 \times 10^{-3} & \boldsymbol{\eta}_{\lambda_2} = (-0.17, 0.99). \end{cases}$$

Thus, at the solution, the cost function is significantly more sensitive to the μ_f -direction rather than the κ_f one. Hence, as $[\nabla^2 J]^{-1}$ is employed, noisy inputs will a priori affect more the reconstruction of the bulk modulus κ_f than the shear one μ_f . Note that both eigenvalues of the Hessian matrix are positive so found the solution is a local minimum.

However, the study of the Hessian matrix is not sufficient to quantify the propagation of uncertainties to the identified parameters. In practice, the uncertainties on the measured effective moduli may vary significantly from one parameter to another. In this context, a possible strategy is to conduct a statistical analysis through Monte Carlo computations, but their cost is often prohibitive when a unique identification is time-expensive. An alternative to quantify the effect of data uncertainties is to conduct a perturbation analysis of the cost function. Consider a data parameter of interest that we denote as $\boldsymbol{\zeta}$. Typically, $\boldsymbol{\zeta}$ can be a subset of $\boldsymbol{\eta}_{\text{eff}}$, which we have previously assumed to be measured, or a parameter considered to be known about a constituent. With a slight abuse of notation, the cost function is now recast as $J(\boldsymbol{\eta}) \equiv J(\boldsymbol{\eta}, \boldsymbol{\zeta})$ and it can be expanded at the first order as

$$J(\boldsymbol{\eta}, \boldsymbol{\zeta} + d\boldsymbol{\zeta}) = J(\boldsymbol{\eta}, \boldsymbol{\zeta}) + \frac{\partial J}{\partial \boldsymbol{\zeta}}(\boldsymbol{\eta}, \boldsymbol{\zeta}) d\boldsymbol{\zeta} + o(\|d\boldsymbol{\zeta}\|).$$

Let $\boldsymbol{\eta}_{\text{id}}$ be an identified minimum of the unperturbed cost function $\boldsymbol{\eta} \mapsto J(\boldsymbol{\eta}, \boldsymbol{\zeta}_{\text{ref}})$, where $\boldsymbol{\zeta}_{\text{ref}}$ is a reference data value for the parameter $\boldsymbol{\zeta}$, and $\tilde{\boldsymbol{\eta}}_{\text{id}}$ be a minimum relative to a perturbed version $\boldsymbol{\eta} \mapsto J(\boldsymbol{\eta}, \tilde{\boldsymbol{\zeta}}_{\text{ref}})$, given $\tilde{\boldsymbol{\zeta}}_{\text{ref}} = \boldsymbol{\zeta}_{\text{ref}} + d\boldsymbol{\zeta}_{\text{ref}}$. It is further assumed that $\tilde{\boldsymbol{\eta}}_{\text{id}}$ can be linearized as

$$\tilde{\boldsymbol{\eta}}_{\text{id}} = \boldsymbol{\eta}_{\text{id}} + \delta\boldsymbol{\eta}_{\text{id}} \quad \text{with} \quad \|\delta\boldsymbol{\eta}_{\text{id}}\| \ll 1.$$

Considering the asymptotic expansion of the gradients of the cost functions above, truncated at the first order in the perturbation, since $\partial J(\boldsymbol{\eta}_{\text{id}}, \boldsymbol{\zeta}_{\text{ref}})/\partial \boldsymbol{\eta} = \mathbf{0}$ and $\partial J(\tilde{\boldsymbol{\eta}}_{\text{id}}, \tilde{\boldsymbol{\zeta}}_{\text{ref}})/\partial \boldsymbol{\eta} = \mathbf{0}$, we finally get:

$$\delta\boldsymbol{\eta}_{\text{id}} = - \left[\frac{\partial^2 J(\boldsymbol{\eta}_{\text{id}}, \boldsymbol{\zeta}_{\text{ref}})}{\partial \boldsymbol{\eta}^2} \right]^{-1} \frac{\partial^2 J(\boldsymbol{\eta}_{\text{id}}, \boldsymbol{\zeta}_{\text{ref}})}{\partial \boldsymbol{\eta} \partial \boldsymbol{\zeta}} d\boldsymbol{\zeta}_{\text{ref}}. \quad (36)$$

Figure 7 displays the reconstruction deviations for the fiber properties κ_f and μ_f in relation to perturbations of various data parameters $\boldsymbol{\zeta}$ of interest: composite moduli $E_{\ell, \text{eff}}$ and $\mu_{\ell, \text{eff}}$ and matrix moduli κ_m and μ_m . The lines represent approximations derived from the linearized formula (36), whereas exact identifications yield discrete points by minimizing (35) through full-field computations. In general, the effects of these deviations are effectively captured by the linearized estimation. However, when output deviations exceed 50%, the influence of non-linearities becomes substantial. For instance, applying a +5% perturbation to μ_m resulted in no solution, with κ_f approaching an infinite value.

While the sensitivity maps in Figure 6 illustrate the impact of microscale parameters on macroscale ones, these sensitivities alone do not fully account for the sensitivities of J , *i.e.* quantify the output deviation for a given input deviation. For instance, the phase sensitivities suggest that the composite modulus $\mu_{\ell, \text{eff}}$ is independent of the bulk moduli of the various phases, see Figure 6 with normalization factor of $\mathcal{O}(10^{-20})$. However, introducing reciprocally a deviation in $\mu_{\ell, \text{eff}}$ results in a significant change in κ_f . This observation stems from the expression in (36), which incorporates the

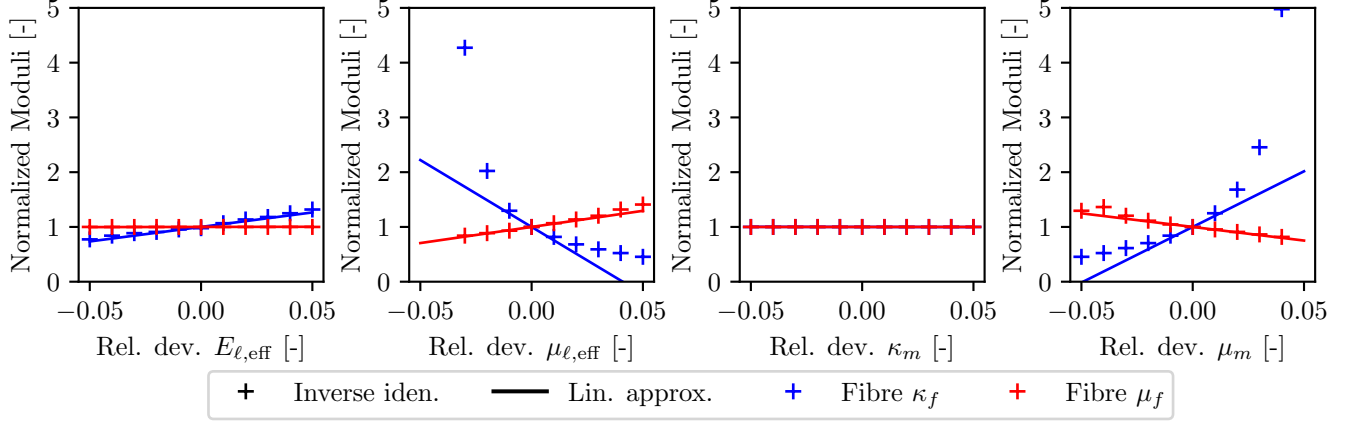


Figure 7: Effects of uncertainties on the identified quantities: solid line are approximations derived from the linearized formula (36). Cross symbols are complete computations without specific approximation. Red: uncertainty of the fiber shear modulus μ_f . Blue: uncertainty of the fiber bulk modulus κ_f .

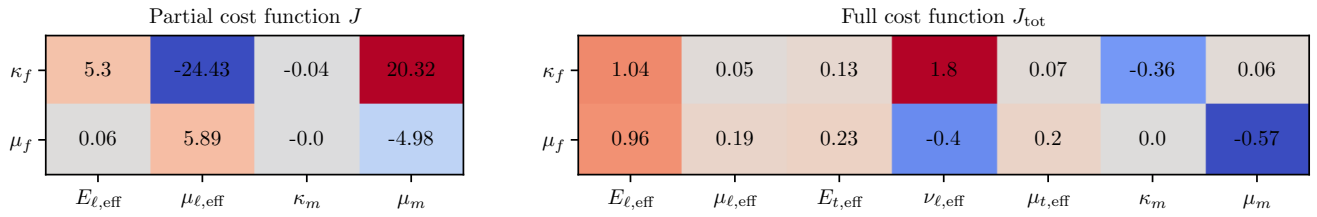


Figure 8: Comparison of the relative sensitivities for two cost functions J and J_{tot} that include 2 and 5 out of 5 composite moduli, respectively. For example: the value of 5.3 linking $E_{\ell,eff}$ to κ_f means that the uncertainty on κ_f is equal to the uncertainty on $E_{\ell,eff}$ multiplied by 5.3.

derivatives of J , where $E_{\ell,\text{eff}}$ and $\mu_{\ell,\text{eff}}$ are interrelated. If the results of Figure 6 are relatively predictable, foreseeing the sensitivity of J is challenging, and the linearized uncertainties are relevant and inexpensive tools to assess them.

Predicting the uncertainties in the cost function poses significant challenges. Thus, the proposed method advocates for selecting an appropriate cost function (or appropriate set of experiments) for a given set of parameters to be identified. In the current example, the cost function J (as defined in (35)) considers only two out of five parameters of the transverse isotropic composite. An alternative approach involves all known composite moduli to define a new cost function J_{tot} , expressed as follows:

$$J_{\text{tot}}(\boldsymbol{\eta}) = J(\boldsymbol{\eta}) + \left(\frac{E_{t,\text{eff}}(\boldsymbol{\eta}) - E_{t,\text{eff}}^{\text{d}}}{E_{t,\text{eff}}^{\text{d}}} \right)^2 + \left(\frac{\nu_{\ell,\text{eff}}(\boldsymbol{\eta}) - \nu_{\ell,\text{eff}}^{\text{d}}}{\nu_{\ell,\text{eff}}^{\text{d}}} \right)^2 + \left(\frac{\mu_{t,\text{eff}}(\boldsymbol{\eta}) - \mu_{t,\text{eff}}^{\text{d}}}{\mu_{t,\text{eff}}^{\text{d}}} \right)^2$$

where, $E_{t,\text{eff}}$ represents the transverse Young modulus, $\nu_{\ell,\text{eff}}$ the longitudinal Poisson ratio, and $\mu_{t,\text{eff}}$ the transverse shear modulus. It is checked that the solution found with J_{tot} is closed to the previous one, regarding to the stopping criterion. The sensitivities of the two cost functions are illustrated in Figure 8. The values are normalized *w.r.t.* the moduli, meaning they give the linearized slopes depicted in Figure 7. Large values reflect a poor choice of experiments used to identify unknown parameters κ_f and μ_f . It is important to note that the sensitivities of J_{tot} are calculated using (36) adapted to the new cost function. The sensitivities of J_{tot} are significantly enhanced due to the inclusion of redundant information in the cost function. However, some sensitivities may also increase. Measuring all composite parameters can be cumbersome, and not all may be essential for the cost function. Further exploration of the relevant parameters to include in the cost function (along with appropriate weighting) is advisable to ensure the low sensitivity of identified parameters' and facilitate a manageable experimental campaign.

Ultimately, this linearized tool is not recommended for a final quantification of uncertainties in an identification process. A Monte Carlo study would yield more accurate results, particularly in capturing potential non-linearities that are not described with that current approach.

5. Identification of viscoelastic phases

The previous identification framework can be extended to viscoelastic materials, a problem that we address in this section. The model is first introduced, then the identification method is discussed on an illustrative numerical example.

5.1. Linear viscoelastic problem

Linear viscoelastic materials are characterized by a time-dependent constitutive relation which can be written by means of the Stieltjes convolution:

$$\boldsymbol{\sigma}(\mathbf{x}, t) = \int_0^t \mathbf{C}(\mathbf{x}, t - \tau, \boldsymbol{\eta}) \, \text{d}\boldsymbol{\varepsilon}(\mathbf{x}, \tau) \quad (37)$$

where $\mathbf{C}(\mathbf{x}, t, \boldsymbol{\eta})$ is the viscoelastic relaxation tensor (Christensen, 1982), which depends on a set $\boldsymbol{\eta}$ of parameters of interest, and t is the time variable. Although we could consider the viscoelastic time-domain response of the composite, we have chosen here to work equivalently from the harmonic response in order to avoid costly time-dependent computations. The effective behaviour of linear viscoelastic composites whose constituents follow a law of type (37) can be obtained using

the correspondence principle, see (Hashin, 1965). This principle is based on the Laplace–Carson transform $g^*(p)$ of a function $g(t)$ given by:

$$g^*(p) = p \int_0^{+\infty} g(t) \exp(-pt) dt,$$

where p is the (complex) Laplace variable, which transforms the Stieltjes convolution into a simple product:

$$\boldsymbol{\sigma}^*(\mathbf{x}, p) = \mathbf{C}^*(\mathbf{x}, p, \boldsymbol{\eta}) \boldsymbol{\varepsilon}^*(\mathbf{x}, p)$$

In the Laplace–Carson space, the linear viscoelastic law become an “elasticity-like” law associated with the complex moduli $\mathbf{C}^*$. The special case where p is purely complex, of the form $p = i\omega$, corresponds to the steady state response of the material to harmonic loading at frequency ω . Such experiments, called dynamic mechanical analysis (DMA), are commonly used to identify the behaviour of linear viscoelastic materials, see (Lakes, 2004). In this section, DMA will be used to obtain and quantify the effective response of linear viscoelastic composites, see (El Archi et al., 2022). As a result, the application of the proposed method to the case of linear viscoelastic materials is similar to the case of elastic materials, treated in the previous section, with the difference that the effective moduli used to construct the cost function are non complex-valued. These effective moduli are obtained by solving the equilibrium problem:

$$\begin{cases} \boldsymbol{\varepsilon}_\eta^*(\mathbf{x}, i\omega) = \mathbf{E}^* + \boldsymbol{\varepsilon}[\mathbf{u}_\eta^*](\mathbf{x}, i\omega), & \mathbf{u}_\eta^* \text{ periodic on } \partial\Omega, \\ \boldsymbol{\sigma}_\eta^*(\mathbf{x}, i\omega) = \mathbf{C}^*(\mathbf{x}, i\omega, \boldsymbol{\eta}) \boldsymbol{\varepsilon}_\eta^*(\mathbf{x}, i\omega), \\ \operatorname{div} \boldsymbol{\sigma}_\eta^*(\mathbf{x}, i\omega) = \mathbf{0}, & \boldsymbol{\sigma}_\eta^* \mathbf{n} \text{ anti-periodic on } \partial\Omega. \end{cases} \quad (38)$$

This problem is equivalent to (1) and can be solved using the same techniques. In this framework, the computation of the derivatives (26) and (28) remains valid for constitutive parameters $\boldsymbol{\eta}$ of interest that are real-valued.

5.2. Example setting

The example treated in the following considers a similar composite (fibre+matrix) as in the previous example. However, we now consider a viscoelastic matrix and, thus, a viscoelastic composite. The objective is to identify the viscoelastic parameters of the matrix, with the fiber behaviour being known and the viscoelastic response of the composite being only partially measured.

The fibres properties are the same as in the previous example, see Table 1. The matrix is assumed to be governed by a generalized Maxwell behaviour with viscoelastic tensor:

$$\mathbf{C}_m^*(p) = 3\kappa_m^*(p)\mathbf{J} + 2\mu_m^*(p)\mathbf{K},$$

with the bulk modulus being characterized by one purely elastic parameter and N_b viscous branches as

$$\kappa_m^*(p) = \kappa_\infty + \sum_{i=1}^{N_b} \frac{\kappa_i p}{p + \tau_{\kappa,i}^{-1}},$$

with κ_∞ the purely relaxed moduli and $\{\tau_{\kappa,i}\}$ being some characteristic relaxation times with the associated moduli $\{\kappa_i\}$. The shear modulus $\mu_m^*(p)$ is assumed to retain a similar form, in terms of some associated parameters, with the appropriate changes in notation. To generate the synthetic

data, the number of viscous branches is set to $N_b = 3$ and all parameters are given Table 2. In practice, polymer matrices can be typically modelled with 10–20 Maxwell branches so as to capture a broad relaxation spectrum. Yet, for clarity and simplicity, we use only three branches (synthetic material) to focus on methodological aspects without compromising conceptual understanding. The targeted characteristic times are different for the bulk or shear modulus and two are closed and one is further away.

κ_∞^*	κ_1^*	$\tau_{\kappa,1}^*$	κ_2^*	$\tau_{\kappa,2}^*$	κ_3^*	$\tau_{\kappa,3}^*$
2.22	1.67	0.25	2.78	0.95	1.67	1.4
μ_∞^*	μ_1^*	$\tau_{\mu,1}^*$	μ_2^*	$\tau_{\mu,2}^*$	μ_3^*	$\tau_{\mu,3}^*$
0.89	0.22	1.8	0.45	8.2	0.22	9.8

Table 2: Reference and targeted viscoelastic matrix. Moduli are given in GPa and characteristic time in s.

The considered known quantities are the fibers properties as well as the macroscopic complex transverse Young's modulus $E_{t,\text{eff}}^{\text{d}\star}$ and the longitudinal shear modulus $\mu_{\ell,\text{eff}}^{\text{d}\star}$ for some frequencies $\{\omega_i\}$. These complex moduli can be classically measured with DMA tensile tests performed on laminates $[90^\circ]$, which gives directly $E_{t,\text{eff}}^{\text{d}\star}$, and $[+45^\circ, -45^\circ]$ to obtain $\mu_{\ell,\text{eff}}^{\text{d}\star}$.

5.3. Reconstruction of viscoelastic parameters

5.3.1. Problem setting

In the context described above, we aim at identifying the properties of the matrix. In particular, given the measured complex moduli of the composite, we aim at identifying the matrix in the form of Prony series:

$$\tilde{\kappa}_m^*(p) = \tilde{\kappa}_\infty + \sum_{i=1}^{\tilde{N}_b} \frac{\tilde{\kappa}_i p}{p + \tilde{\tau}_{\kappa,i}^{-1}}$$

and similarly with $\tilde{\mu}_m^*$. Therefore, the unknowns of the problem are described by the vector:

$$\boldsymbol{\eta} = (\tilde{\kappa}_\infty, \{\tilde{\kappa}_i\}_{i=1,\dots,\tilde{N}_b}, \{\tilde{\tau}_{\kappa,i}\}_{i=1,\dots,\tilde{N}_b}, \tilde{\mu}_\infty, \{\tilde{\mu}_i\}_{i=1,\dots,\tilde{N}_b}, \{\tilde{\tau}_{\mu,i}\}_{i=1,\dots,\tilde{N}_b}). \quad (39)$$

with the arbitrary choice $\tilde{N}_b = 5$, to be compared with the targeted number of branches $N_b^* = 3$.

As previously with the consideration of (35), identification is achieved by minimizing a cost function over $\{\omega_i\}_{i \in [1, N_\omega]}$ frequencies as follows

$$\min_{\boldsymbol{\eta}} J(\boldsymbol{\eta}) = \min_{\boldsymbol{\eta}} \frac{1}{N_\omega} \sum_{i=1}^{N_\omega} \frac{|E_{t,\text{eff}}^*(\boldsymbol{\eta}, \omega_i) - E_{t,\text{eff}}^{\text{d}\star}(\omega_i)|^2}{|E_{t,\text{eff}}^{\text{d}\star}(\omega_i)|^2} + \frac{|\mu_{\ell,\text{eff}}^*(\boldsymbol{\eta}, \omega_i) - \mu_{\ell,\text{eff}}^{\text{d}\star}(\omega_i)|^2}{|\mu_{\ell,\text{eff}}^{\text{d}\star}(\omega_i)|^2}. \quad (40)$$

The choice of identification frequencies $\{\omega_i\}_{i \in [1, N_\omega]}$ involved in the cost function are chosen as $\omega_1 \rightarrow 0$ (numerical zero) and thirteen are evenly distributed in log scale between 10^{-2} and 10 s^{-1} . The choice of the number of $\{\omega_i\}$ will be investigated.

Remark 6. An alternative, would be to identify first the characteristic times of the composite and, based on the collocation method proposed by (Schapery, 2014), choose the frequencies accordingly.

The complex problem (38) is simulated using the FFT-based homogenization method. The considered microstructure is, this time, a composite with fibers in hexagonal stacking. Given the periodicity of the microstructure, this allows us to consider a representative cell containing only two fibers, which is discretized into $128 \times 128 \times 1$ pixels, see Figure 4b. This choice is made to reduce the numerical cost. As for the previous example, synthetic data are generated using a different solver scheme than this used in the inversion, namely that of (Eyre and Milton, 1999). The parameters in $\boldsymbol{\eta}$ are search positive, with an exponential function guaranteeing this at each step.

5.3.2. Initialization of the reconstruction

In order to solve the problem (40), the BFGS algorithm is chosen for its speed and efficiency in the previous example. One may chose a Newton algorithm that necessitates to solve the additional cell-problem (21). As discussed, a suitable initialization of such a scheme is important to obtain satisfying reconstructions. When $t \rightarrow 0$ or $t \rightarrow \infty$, the visco-elastic problem becomes elastic, and identifications as in Section 4 can be employed to identify κ_0 and κ_∞ defined by

$$\kappa_0 = \lim_{p \rightarrow \infty} \kappa_m^*(p) = \lim_{t \rightarrow 0} \kappa_m(t), \quad \kappa_\infty = \lim_{p \rightarrow 0} \kappa_m^*(p) = \lim_{t \rightarrow \infty} \kappa_m(t),$$

and respectively for μ_0 and μ_∞ . This allows to remove $\tilde{\kappa}_\infty$ and $\tilde{\mu}_\infty$ from the $\boldsymbol{\eta}$ defined in (39). For the initialization, the characteristic times $\{\tilde{\tau}_{\kappa,i}\}$ and $\{\tilde{\tau}_{\mu,i}\}$ are chosen evenly distributed in log scale between 0.1 and 10 s. The modulus of each branch is initialized as follows:

$$\tilde{\kappa}_i = \frac{\tilde{\kappa}_0 - \tilde{\kappa}_\infty}{\tilde{N}_b}$$

and similarly for the shear moduli $\{\tilde{\mu}_i\}$.

5.4. Identification results

The composite behaviour, along with the reference matrix, the initialization matrix, and the identified matrix, are illustrated in Figure 9. As expected, based on the initialization process, the initialization matrix effectively captures the behaviour at both zero and infinity frequencies. The identified matrix demonstrates excellent composite behaviour, with comparable residual errors between the two moduli. The matrices responses are presented in the frequency domain in Figure 10. Similar to the composite results, the error between the identified and reference matrices is relatively low. However, there are noticeable discrepancies regarding the moduli of the viscous branches, as shown in Figure 11. The moduli and characteristic times are overall correctly identified, highlighting the method efficiency. The shear parameters are accurately identified both in terms of weight and characteristic times. In some instances, branches with similar characteristic times, τ_i , may combine to form a single branch, but close τ_i in the reference matrix are still successfully identified. Identifying the bulk modulus is less effective, exhibiting more significant deviations in κ_i and τ_i . It is important to note that identifying Prony's series is an ill-posed problem (Jalocha et al., 2015) with known issues regarding multiple solutions. Here, such parameter deviations have minimal impact on the complex moduli of the matrix in the frequency domain, *i.e.* different Prony models can lead to a similar response.

The sensitivities of the identified properties to input parameters are shown in Figure 12. These results are computed with the reference matrix (Table 2) composed of 2×3 branches by finite differences of gradients. Note that the values are not normalized. The bulk moduli and the characteristic times of the shear branches are the most sensitive to input parameters. Because the frequencies are

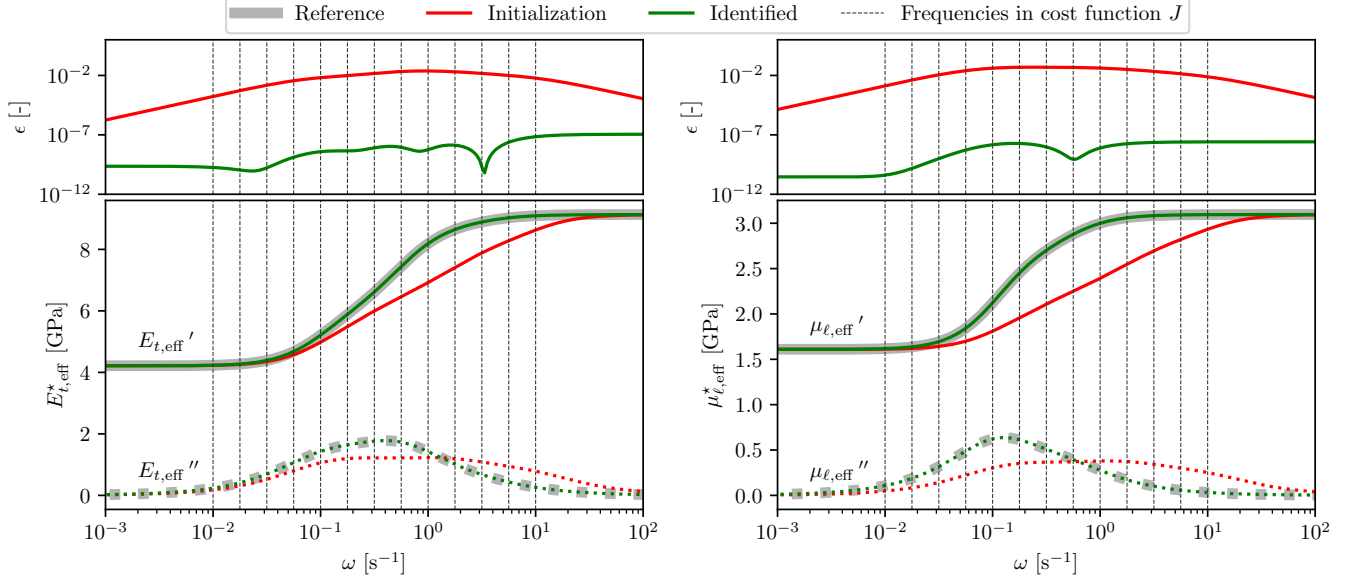


Figure 9: Complex moduli of the composite in the frequency space, split into real and imaginary parts, $E_{t,\text{eff}}^* = E_{t,\text{eff}}' + iE_{t,\text{eff}}''$ and $\mu_{t,\text{eff}}^* = \mu_{t,\text{eff}}' + i\mu_{t,\text{eff}}''$. In top panels, ϵ denotes the relative error of the complex moduli relative to the reference one.

sorted from the smallest to the largest, the sensitivities are greater in the middle range because of a significant change occurring in the material behaviour, which is crucial for the identification.

The impact of the number of viscous branches $\tilde{N}_b$ in the identified matrix and the number of frequencies N_ω in the cost function are also investigated. The resulting errors in matrix moduli compared to the reference are reported in Figure 13. With $N_\omega = 12$, the error quickly converged at $\tilde{N}_b = 4$, and increasing the number of branches beyond this point does not enhance the identification process. While the reference matrix has three branches, it is noteworthy that the error with three branches is higher due to possible local minima depending on the initialization. In general, while increasing the number of branches could result in an over-parameterized model, post-simplifications may be considered, such as merging branches with similar characteristic times or omitting branches with low weights. Additionally, it is important to mention that in the Laplace–Carson space, increasing the number of branches has minimal impact on computation efficiency and, consequently, on the speed of the identification algorithm.

Concerning the number of frequencies N_ω in the cost function, we observed that the error converges for $N_\omega = 5$ (with $\tilde{N}_b = 5$). Although increasing this number does not enhance the numerical accuracy of the identified parameters, adding more frequencies in the context of experimental data can mitigate the impact of noise, akin to a regression analysis. However, it is important to note that increasing N_ω significantly affects the identification speed, as the complex problem must be solved for each additional frequency.

6. Conclusion

This study focuses on identifying the individual microscale properties of a composite constituents from macroscopic response data and the knowledge of the complementary subset of microscale material parameters. Such parameter identifications are achieved by minimizing a cost function with first and second-order gradient-based algorithms. To do so, the needed cost function derivatives

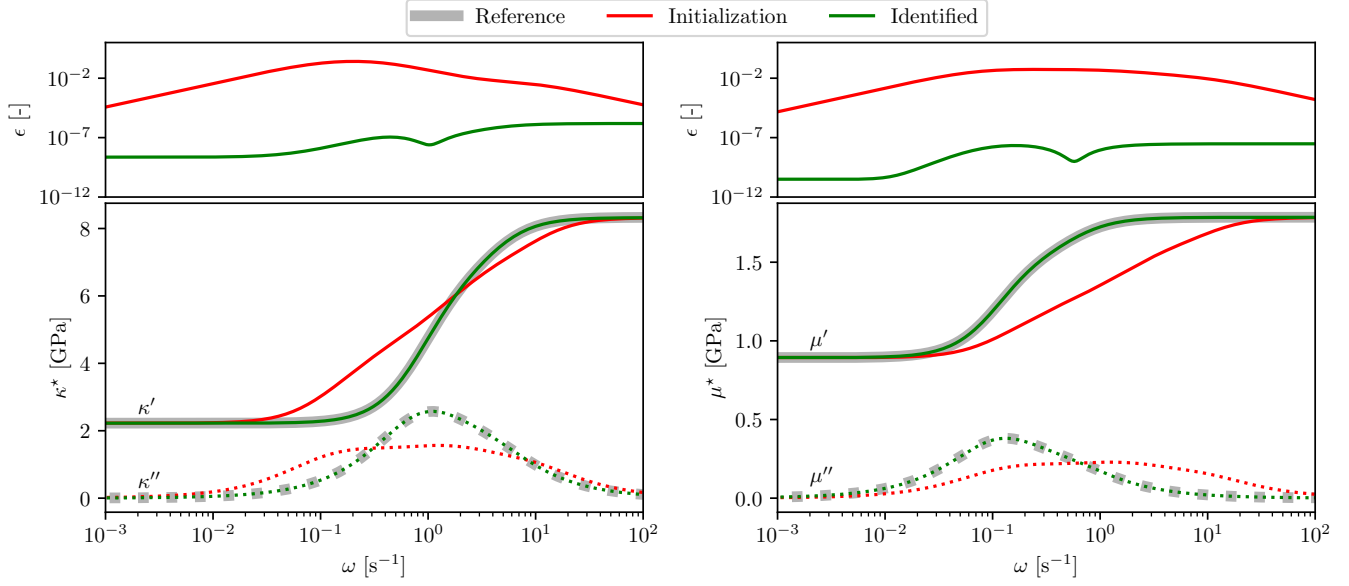


Figure 10: Complex moduli of the matrix in the frequency space, split into real and imaginary parts, $\kappa^* = \kappa' + i\kappa''$ and $\mu^* = \mu' + i\mu''$. In top panels, ϵ denotes the relative error of the complex moduli relative to the reference one.

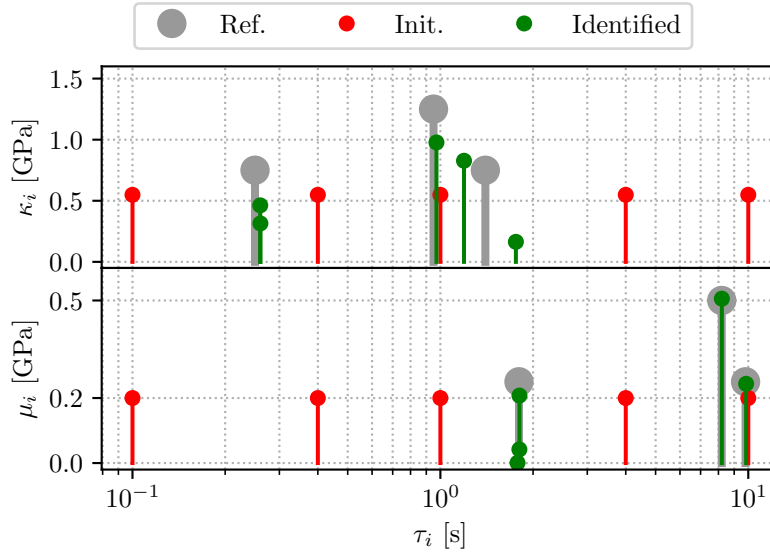


Figure 11: Moduli of the viscous branches and their respective characteristic times.

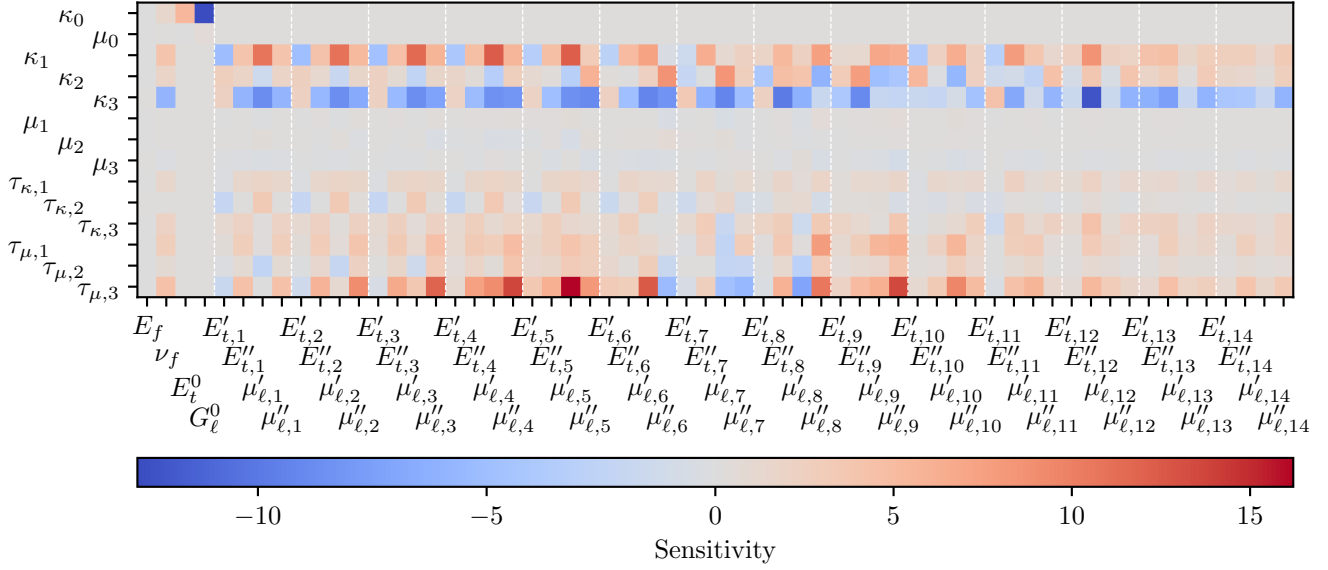


Figure 12: Sensitivities of the identified parameters to the input parameters of the matrix (see relation (36)). X'_i and X''_i denote respectively the real and imaginary part of the complex modulus X at ω_i . The abscissa ticks correspond to effective quantities; the x_{eff} subscript is omitted for clarity.

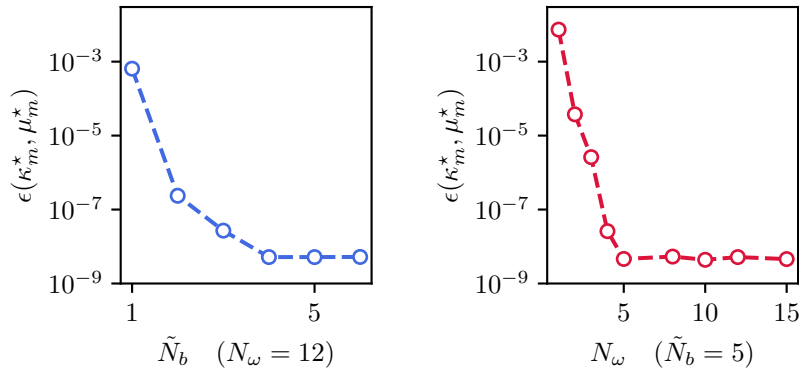


Figure 13: Error in the matrix complex moduli κ^* and μ^* as functions of the number of viscous branches $\tilde{N}_b$ in the identified matrix, and the number of frequencies N_ω in the cost function. The error $\epsilon(\kappa_m^*, \mu_m^*)$ is computed by integrating in log scale between $\omega = 10^{-2}$ and 10^2 s^{-1} on both (summed) κ^* and μ^* .

are computed from the continuous mechanical model considered, i.e. before any discretization step, and the associated computations required are investigated. The following main conclusions can be drawn from this study:

- Considering an energy-based approach optimizes the number of cell problems to be solved to compute the cost function derivatives. More precisely, the computation of the gradient becomes direct, necessitating only the solution fields obtained during standard homogenization computations. This result makes the BFGS algorithm particularly efficient since a new estimate of the Hessian matrix is readily available at each step. The proposed approach is applicable to composites with any number of phases, without requiring methodological changes. Two-phase systems were considered in the examples for clarity and practicality, while extensions to multi-phase composites are left for case-specific future studies.
- The first example considered aims at identifying moduli of elastic fibers within a composite, from synthetic data. The identification is successful, and a sensitivity analysis allows to determine that the bulk moduli is indirectly very sensitive to the shear modulus of the matrix and the longitudinal young modulus of the composite. Sensitivity maps are drawn, showing high local sensitivity in regions of the matrix where fibres are close to one another. In the context of fibre-reinforced composites, it would be relevant to address the case of transverse isotropic fibres, such as carbon fibres, using the method presented here, which will be the subject of a future study.
- In the second example proposed, viscoelastic properties of the matrix are identified for the same type of fiber reinforced composite. The complex effective transverse Young’s and longitudinal shear moduli are included in the cost function. The identified matrix is close to the reference matrix, with barely any difference in their complex moduli. However, some discrepancies are observed for the bulk modulus when examining the viscous branches individually.

Through the examples, various issues and corresponding mitigation strategies were highlighted. Because of the inherent ill-posed nature of the problem, no conclusions can be drawn regarding the quality of reconstructions for any material configuration. Factors like the phase contrast, the microstructure geometry, and which parameters are known or unknown may affect the outcome. We therefore recommend that each case be studied specifically using the tools provided here in order to anticipate potential difficulties before proceeding with identification. These insights allow us to outline key guidelines that can inform the identification process in specific, case-dependent contexts:

- Determine a first guess for the targeted constitutive properties using, for example, mean-field estimates or low-fidelity computations.
- Perform cell problems computations on the RVE to determine the gradient and Hessian of suitable cost functions. Apply a linear sensitivity analysis, Eq. (34), to assess parameter dependencies, and use the corresponding uncertainty analysis, Eq. (36), to build a robust cost function and, consequently, to determine the required input data. Based on these insights, design the necessary experiments and implement appropriate measures to minimize the propagation of uncertainties.
- Using available data, ideally from best practice tests, identify the targeted parameters using BFGS or Newton’s algorithm depending on the number of unknowns.
- Determine the final uncertainties of the identified properties using linearized approximations of the uncertainties.

- Train/make a fast-to-compute model (*e.g.* using a Gaussian Process Regression) to perform a detailed (nonlinear) quantification of the uncertainties using a Monte-Carlo approach.

In summary, strain fields obtained from direct homogenization are used in inverse homogenization problems to compute derivatives of cost functions, estimate the uncertainties in the identified microscale parameters, and pinpoint the critical variables on which to act to reduce the errors in the identification process.

7. Author contributions

Robin Valmalette: Investigation, Methodology, Software, Validation, Visualization, Writing – original draft, Writing – review and editing. **Cédric Bellis:** Investigation, Methodology, Validation, Writing – review and editing. **Noël Lahellec:** Investigation, Methodology, Validation, Writing – review and editing. **Christian Hochard:** Validation, Writing – review and editing.

8. Funding sources

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors

References

- Audoit, J., Rivière, L., Dandurand, J., Lonjon, A., Dantras, E., Lacabanne, C., 2019. Thermal, mechanical and dielectric behaviour of poly(aryl ether ketone) with low melting temperature. *Journal of Thermal Analysis and Calorimetry* 135, 2147–2157. doi:[10.1007/s10973-018-7292-x](https://doi.org/10.1007/s10973-018-7292-x).
- Bellis, C., Moulinec, H., Suquet, P., 2020. Eigendecomposition-based convergence analysis of the Neumann series for laminated composites and discretization error estimation. *International Journal for Numerical Methods in Engineering* 121, 201–232. doi:[10.1002/nme.6206](https://doi.org/10.1002/nme.6206).
- Bellis, C., Suquet, P., 2019. Geometric Variational Principles for Computational Homogenization. *Journal of Elasticity* 137, 119–149. doi:[10.1007/s10659-018-09713-9](https://doi.org/10.1007/s10659-018-09713-9).
- Blackketter, D.M., Upadhyaya, D., King, T.R., 1993. Micromechanics prediction of the transverse tensile strength of carbon fiber/epoxy composites: The influence of the matrix and interface. *Polymer Composites* 14, 437–446. doi:[10.1002/pc.750140511](https://doi.org/10.1002/pc.750140511).
- Bobeth, M., Diener, G., 1986. Field fluctuations in multicomponent mixtures. *Journal of the Mechanics and Physics of Solids* 34, 1–17. doi:[https://doi.org/10.1016/0022-5096\(86\)90002-5](https://doi.org/10.1016/0022-5096(86)90002-5).
- Breite, C., Melnikov, A., Turon, A., De Morais, A., Otero, F., Mesquita, F., Costa, J., Mayugo, J., Guerrero, J., Gorbatiikh, L., McCartney, L., Hajikazemi, M., Camanho, P., Tavares, R., Lomov, S., Pimenta, S., Van Paepegem, W., Swolfs, Y., 2021. Blind benchmarking of seven longitudinal tensile failure models for two virtual unidirectional composites. *Composites Science and Technology* 202, 108555. doi:[10.1016/j.compscitech.2020.108555](https://doi.org/10.1016/j.compscitech.2020.108555).
- Burczyński, T., Kuś, W., 2008. Identification of material properties in multi-scale modelling. *Journal of Physics: Conference Series* 135, 012025. doi:[10.1088/1742-6596/135/1/012025](https://doi.org/10.1088/1742-6596/135/1/012025).

- Chen, Y., Vasiukov, D., Gélébart, L., Park, C.H., 2019. A FFT solver for variational phase-field modeling of brittle fracture. *Computer Methods in Applied Mechanics and Engineering* 349, 167–190. doi:[10.1016/j.cma.2019.02.017](https://doi.org/10.1016/j.cma.2019.02.017).
- Christensen, R.M., 1982. Chapter I - Viscoelastic Stress Strain Constitutive Relations, in: Christensen, R.M. (Ed.), *Theory of Viscoelasticity* (Second Edition). Academic Press, pp. 1–34. doi:[10.1016/B978-0-12-174252-2.50005-3](https://doi.org/10.1016/B978-0-12-174252-2.50005-3).
- Cornaggia, R., Bellis, C., 2020. Tuning effective dynamical properties of periodic media by fft-accelerated topological optimization. *International Journal for Numerical Methods in Engineering* 121, 3178–3205.
- Diebels, S., Scheffer, T., Schuster, T., Wewior, A., 2018. Identifying Elastic and Viscoelastic Material Parameters by Means of a Tikhonov Regularization. *Mathematical Problems in Engineering* 2018, 1895208. doi:[10.1155/2018/1895208](https://doi.org/10.1155/2018/1895208).
- Donadon, M.V., Falzon, B.G., Iannucci, L., Hodgkinson, J.M., 2007. A 3-D micromechanical model for predicting the elastic behaviour of woven laminates. *Composites Science and Technology* 67, 2467–2477. doi:[10.1016/j.compscitech.2006.12.019](https://doi.org/10.1016/j.compscitech.2006.12.019).
- El Archi, Y., Lahellec, N., Lejeunes, S., Jouan, A., Tranquart, B., 2022. Multiscale simulation and experimental analysis of damping in cfrp structures containing rubber. *Composite Structures* 289, 115456.
- Eyre, D., Milton, G., 1999. A Fast Numerical Scheme for Computing the Response of Composites Using Grid Refinement. *The European Physical Journal Applied Physics* 6. doi:[10.1051/epjap:1999150](https://doi.org/10.1051/epjap:1999150).
- Fedele, R., Maier, G., Whelan, M., 2006. Stochastic calibration of local constitutive models through measurements at the macroscale in heterogeneous media. *Computer Methods in Applied Mechanics and Engineering* 195, 4971–4990. doi:[10.1016/j.cma.2005.07.026](https://doi.org/10.1016/j.cma.2005.07.026).
- Feyel, F., Chaboche, J.L., 2000. FE2 multiscale approach for modelling the elastoviscoplastic behaviour of long fibre SiC/Ti composite materials. *Computer Methods in Applied Mechanics and Engineering* 183, 309–330. doi:[10.1016/S0045-7825\(99\)00224-8](https://doi.org/10.1016/S0045-7825(99)00224-8).
- Fish, J., Ghouali, A., 2001. Multiscale analytical sensitivity analysis for composite materials. *International Journal for Numerical Methods in Engineering* 50, 1501–1520. doi:[10.1002/1097-0207\(20010228\)50:6<1501::AID-NME84>3.0.CO;2-0](https://doi.org/10.1002/1097-0207(20010228)50:6<1501::AID-NME84>3.0.CO;2-0).
- Goldberg, R., Kohlman, L., Cater, C., Xiao, X., 2015. Experimental and Numerical Analysis of Triaxially Braided Composites Utilizing a Modified Subcell Modeling Approach.
- Gonçalves, P.T., Arteiro, A., Rocha, N., Pina, L., 2022. Numerical Analysis of Micro-Residual Stresses in a Carbon/Epoxy Polymer Matrix Composite during Curing Process. *Polymers* 14, 2653. doi:[10.3390/polym14132653](https://doi.org/10.3390/polym14132653).
- Gregory, J.R., Spearing, S.M., 2005. Nanoindentation of neat and in situ polymers in polymer-matrix composites. *Composites Science and Technology* 65, 595–607. doi:[10.1016/j.compscitech.2004.09.001](https://doi.org/10.1016/j.compscitech.2004.09.001).

- Hartmann, S., Gilbert, R.R., 2018. Identifiability of material parameters in solid mechanics. *Archive of Applied Mechanics* 88, 3–26. doi:[10.1007/s00419-017-1259-4](https://doi.org/10.1007/s00419-017-1259-4).
- Hashin, Z., 1965. Viscoelastic Behavior of Heterogeneous Media. *Journal of Applied Mechanics* 32, 630–636. doi:[10.1115/1.3627270](https://doi.org/10.1115/1.3627270).
- Huang, Y., Jin, K.K., Ha, S.K., 2008. Effects of fiber arrangement on mechanical behavior of unidirectional composites. *Journal of Composite Materials* 42, 1851–1871. URL: <https://doi.org/10.1177/0021998308093910>, doi:[10.1177/0021998308093910](https://doi.org/10.1177/0021998308093910), arXiv:<https://doi.org/10.1177/0021998308093910>.
- Islam, F., Joannès, S., Bucknell, S., Leray, Y., Bunsell, A., Laiarinandrasana, L., 2020. Investigation of tensile strength and dimensional variation of T700 carbon fibres using an improved experimental setup. *Journal of Reinforced Plastics and Composites* 39, 144–162. doi:[10.1177/0731684419873712](https://doi.org/10.1177/0731684419873712).
- Jalocha, D., Constantinescu, A., Neviere, R., 2015. Revisiting the identification of generalized maxwell models from experimental results. *International Journal of Solids and Structures* 67–68, 169–181. URL: <https://www.sciencedirect.com/science/article/pii/S0020768315001894>, doi:<https://doi.org/10.1016/j.ijsolstr.2015.04.018>.
- Kanit, T., Forest, S., Galliet, I., Mounoury, V., Jeulin, D., 2003. Determination of the size of the representative volume element for random composites: Statistical and numerical approach. *International Journal of Solids and Structures* 40, 3647–3679. doi:[10.1016/S0020-7683\(03\)00143-4](https://doi.org/10.1016/S0020-7683(03)00143-4).
- Katouzian, M., Vlase, S., 2020. Creep Response of Neat and Carbon-Fiber-Reinforced PEEK and Epoxy Determined Using a Micromechanical Model. *Symmetry* 12, 1680. doi:[10.3390/sym12101680](https://doi.org/10.3390/sym12101680).
- Klinge, S., 2012a. Inverse analysis for multiphase nonlinear composites with random microstructure. *International Journal for Multiscale Computational Engineering* 10. doi:[10.1615/IntJMultCompEng.2012002946](https://doi.org/10.1615/IntJMultCompEng.2012002946).
- Klinge, S., 2012b. Parameter identification for two-phase nonlinear composites. *Computers & Structures* 108–109, 118–124. doi:[10.1016/j.compstruc.2012.02.008](https://doi.org/10.1016/j.compstruc.2012.02.008).
- Klinge, S., Steinmann, P., 2015. Inverse analysis for heterogeneous materials and its application to viscoelastic curing polymers. *Computational Mechanics* 55, 603–615. doi:[10.1007/s00466-015-1126-5](https://doi.org/10.1007/s00466-015-1126-5).
- Kreher, W., 1990. Residual stresses and stored elastic energy of composites and polycrystals. *Journal of the Mechanics and Physics of Solids* 38, 115–128. doi:[https://doi.org/10.1016/0022-5096\(90\)90023-W](https://doi.org/10.1016/0022-5096(90)90023-W).
- Lakes, R.S., 2004. Viscoelastic measurement techniques. *Review of Scientific Instruments* 75, 797–810. URL: <https://doi.org/10.1063/1.1651639>.

- M.A. Ghouali, Ghouali, M., Georges Duvaut, Duvaut, G., Sophie Ortola, Ortola, S., Alain Oster, Oster, A., 1998. Local analytical design sensitivity analysis of the forging problem using FEM. *Computer Methods in Applied Mechanics and Engineering* 163, 55–70. doi:[10.1016/S0045-7825\(97\)00313-7](https://doi.org/10.1016/S0045-7825(97)00313-7).
- Merlette, T.C., Diani, J., 2025. Linear viscoelasticity of anisotropic carbon fibers reinforced thermoplastics: From micromechanics to dynamic torsion experiments. *Composites Part B: Engineering* 290, 111931. URL: <https://www.sciencedirect.com/science/article/pii/S1359836824007431>, doi:<https://doi.org/10.1016/j.compositesb.2024.111931>.
- Mishnaevsky, L., Brøndsted, P., 2008. Three-dimensional numerical modelling of damage initiation in unidirectional fiber-reinforced composites with ductile matrix. *Materials Science and Engineering: A* 498, 81–86. doi:[10.1016/j.msea.2007.09.105](https://doi.org/10.1016/j.msea.2007.09.105).
- Miyagawa, H., Sato, C., Mase, T., Drown, E., Drzal, L., Ikegami, K., 2005. Transverse elastic modulus of carbon fibers measured by Raman spectroscopy. *Materials Science and Engineering A* 412, 88–92. doi:[10.1016/j.msea.2005.08.037](https://doi.org/10.1016/j.msea.2005.08.037).
- Moulinec, H., Suquet, P., 1994. A fast numerical method for computing the linear and nonlinear mechanical properties of composites. *Comptes Rendus de l'Académie des sciences. Série II. Mécanique, physique, chimie, astronomie* .
- Moulinec, H., Suquet, P., 1998. A numerical method for computing the overall response of nonlinear composites with complex microstructure. *Computer Methods in Applied Mechanics and Engineering* 157, 69–94. doi:[10.1016/S0045-7825\(97\)00218-1](https://doi.org/10.1016/S0045-7825(97)00218-1).
- Mounier, D., Poilâne, C., Khelifa, H., Picart, P., 2014. Sub-gigahertz laser resonant ultrasound spectroscopy for the evaluation of elastic properties of micrometric fibers. *Ultrasonics* 54, 259–267. doi:[10.1016/j.ultras.2013.06.014](https://doi.org/10.1016/j.ultras.2013.06.014).
- Nocedal, J., Wright, S.J., 2006. *Numerical Optimization*. Springer New York, NY.
- Oskay, C., Fish, J., 2008. On calibration and validation of eigendeformation-based multiscale models for failure analysis of heterogeneous systems. *Computational Mechanics* 42, 181–195. doi:[10.1007/s00466-007-0197-3](https://doi.org/10.1007/s00466-007-0197-3).
- Praud, F., Chatzigeorgiou, G., Meraghni, F., 2021. Fully integrated multi-scale modelling of damage and time-dependency in thermoplastic-based woven composites. *International Journal of Damage Mechanics* 30, 163–195. URL: <https://doi.org/10.1177/1056789520944986>, doi:[10.1177/1056789520944986](https://doi.org/10.1177/1056789520944986), arXiv:<https://doi.org/10.1177/1056789520944986>.
- Qing, H., Mishnaevsky, L., 2009. Unidirectional high fiber content composites: Automatic 3D FE model generation and damage simulation. *Computational Materials Science* 47, 548–555. doi:[10.1016/j.commatsci.2009.09.023](https://doi.org/10.1016/j.commatsci.2009.09.023).
- Schapery, R.A., 2014. A Simple Collocation Method for Fitting Viscoelastic Models to Experimental Data. Technical Report. California Institute of Technology. doi:[10.7907/92J7-G843](https://doi.org/10.7907/92J7-G843).
- Schmidt, U., Mergheim, J., Steinmann, P., 2015. Identification of elastoplastic microscopic material parameters within a homogenization scheme. *International Journal for Numerical Methods in Engineering* 104, 391–407. doi:[10.1002/nme.4933](https://doi.org/10.1002/nme.4933).

- Schmidt, U., Steinmann, P., Mergheim, J., 2016. Two-scale elastic parameter identification from noisy macroscopic data. *Archive of Applied Mechanics* 86, 303–320. doi:[10.1007/s00419-015-1096-2](https://doi.org/10.1007/s00419-015-1096-2).
- Sevenois, R.D.B., Garoz, D., Verboven, E., Spronk, S.W.F., Gilabert, F.A., Kersemans, M., Pyl, L., Van Paepegem, W., 2018. Multiscale approach for identification of transverse isotropic carbon fibre properties and prediction of woven elastic properties using ultrasonic identification. *Composites Science and Technology* 168, 160–169. doi:[10.1016/j.compscitech.2018.09.016](https://doi.org/10.1016/j.compscitech.2018.09.016).
- Soden, P.D., Hinton, M.J., Kaddour, A.S., 1998. Lamina properties, lay-up configurations and loading conditions for a range of fibre-reinforced composite laminates. *Composites Science and Technology* 58, 1011–1022. doi:[10.1016/S0266-3538\(98\)00078-5](https://doi.org/10.1016/S0266-3538(98)00078-5).
- Suquet, P., Ponte Castañeda, P., 1993. Small-contrast perturbation expansions for the effective properties of nonlinear composites. *C. R. Acad. Sci. Paris Ser. II* 317, 1515–1522.
- Swolfs, Y., McMeeking, R.M., Verpoest, I., Gorbatikh, L., 2015. Matrix cracks around fibre breaks and their effect on stress redistribution and failure development in unidirectional composites. *Composites Science and Technology* 108, 16–22. doi:[10.1016/j.compscitech.2015.01.002](https://doi.org/10.1016/j.compscitech.2015.01.002).
- Ureña, A., Rams, J., Escalera, M., Sánchez, M., 2005. Characterization of interfacial mechanical properties in carbon fiber/aluminium matrix composites by the nanoindentation technique. *Composites Science and Technology* 65, 2025–2038. doi:[10.1016/j.compscitech.2005.04.013](https://doi.org/10.1016/j.compscitech.2005.04.013).
- Verpoest, I., Lomov, S., 2005. Virtual textile composites software wisetex: Integration with micro-mechanical, permeability and structural analysis. *Composites Science and Technology* 65, 2563–2574. doi:[10.1016/j.compscitech.2005.05.031](https://doi.org/10.1016/j.compscitech.2005.05.031).
- Wang, B., Fang, G., Tan, X., Liang, J., Ge, J., Liu, S., 2020. Investigation on the longitudinal compressive strength of unidirectional carbon fiber/nanoparticles reinforced polymer composites using FFT-based method. *Composite Structures* 247, 112448. doi:[10.1016/j.compstruct.2020.112448](https://doi.org/10.1016/j.compstruct.2020.112448).
- Younes, R., Hallal, A., Fardoun, F., Chehade, F.H., 2012. Comparative review study on elastic properties modeling for unidirectional composite materials, in: Hu, N. (Ed.), *Composites and Their Properties*. IntechOpen, Rijeka. chapter 17. URL: <https://doi.org/10.5772/50362>, doi:[10.5772/50362](https://doi.org/10.5772/50362).