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Improving FEMU Calibration from a Single Heterogeneous Test through a Data-Driven Approach: An Exploratory Study

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Abstract. Inverse identification of material parameters from experimental data is a long-standing challenge, especially when calibrating complex constitutive models characterized by a large number of parameters. Heterogeneous mechanical tests combined with full-field measurements provide a large amount of information for material parameter identification but lead to high computational costs when used within a Finite Element Model Updating (FEMU) framework. This work presents an exploratory study on the use of surrogate-assisted Bayesian optimization to assess its potential for reducing the number of simulations required for FEMU-based calibration using data from a single notched tensile test. FEMU cost function is applied based on the discrepancy between experimental and numerical strain fields. A Gaussian Process surrogate model is iteratively constructed, and new sets of material parameters are selected using an Expected Improvement criterion. The results are discussed in terms of convergence behaviour and optimization efficiency, providing insight into the suitability of Bayesian optimization for solving inverse identification problems.

Introduction

Accurate calibration of constitutive models is a key requirement for reliable numerical prediction of material behaviour in metal forming and structural applications. Advanced material models, particularly those accounting for nonlinear hardening and plastic anisotropy, typically involve a large number of parameters whose identification requires experimental data that are sufficiently rich to excite multiple deformation states. Traditional identification strategies rely on series of quasi-homogeneous mechanical tests performed under different loading paths and orientations. While effective, such approaches are experimentally demanding and time-consuming.

In recent years, heterogeneous mechanical tests have emerged as a promising alternative, as they enable the activation of a wide range of strain and stress states within a single experiment. When combined with full-field measurement techniques, such as Digital Image Correlation (DIC), these tests provide spatially rich datasets that can significantly enhance the identifiability of constitutive parameters. The use of heterogeneous specimens and full-field data within inverse identification frameworks has been extensively investigated, including previous contributions by the authors, which demonstrated the potential of notched and topology-optimized specimens for full-field FEMU-based material calibration [1-3].

Among inverse strategies, the Finite Element Model Updating (FEMU) [4] approach has been widely adopted for material parameter identification using full-field data. FEMU consists of iteratively updating model parameters to minimize the discrepancy between experimental measurements and finite element predictions. Despite its effectiveness, FEMU-based identification remains computationally expensive, particularly when dealing with high-dimensional parameter spaces and full-field cost functions, as each iteration requires a complete finite element simulation.

More recently, Machine Learning-based (ML) approaches have been proposed as alternatives to classical FEMU, aiming to directly infer material parameters from experimental data without repeated finite element simulations [5, 6]. While these approaches show promising results, they often require large training datasets and may compromise physical interpretability or direct consistency with established finite element models.

To address these limitations, surrogate-assisted optimization techniques have gained increasing attention. In particular, Bayesian Optimization (BO) provides an efficient framework for optimizing expensive black-box functions by combining a probabilistic surrogate model with an acquisition strategy that balances exploration and exploitation. Bayesian optimization has been successfully applied to a wide range of optimization problems in computational mechanics and related fields, demonstrating its ability to reduce the number of costly model evaluations required to reach satisfactory solutions [7, 8]. However, to the best of the authors' knowledge, only a limited number of recent studies have applied Bayesian optimization to FEMU-based material parameter identification [9, 10], and its use in conjunction with heterogeneous mechanical tests remains largely unexplored.

In this context, the present work does not seek to replace FEMU, but rather to enhance it by leveraging machine learning concepts in the form of surrogate-assisted Bayesian optimization. This contribution builds upon previous work on heterogeneous mechanical tests, full-field experimental measurements and FEMU by introducing a data-driven optimization layer on top of a physically grounded FEMU framework. Specifically, the present study investigates the potential of Bayesian optimization coupled with FEMU to improve the efficiency and robustness of material parameter identification using data from a single notched specimen tensile test. The cost function is defined within FEMU framework as the discrepancy between experimental and numerical strain fields, condensed into a scalar value. A Gaussian Process surrogate model is iteratively trained using FEMU evaluations, enabling the adaptive selection of new parameter sets through an acquisition strategy. The proposed framework is evaluated in an exploratory manner, with particular emphasis on convergence behaviour, stability, and the quality of the identified parameters, thereby providing insight into the suitability of Bayesian optimization for reducing the computational burden associated with full-field FEMU calibration while preserving accuracy in reproducing experimentally observed strain fields.

Notched test: experimental setup and numerical model

The present study is based on the notched specimen designed to promote heterogeneous deformation states, including pronounced strain gradients and strain localization in the notch region. Such heterogeneity makes this test particularly interesting and has been extensively investigated in previous works [11]. The experimental procedures and numerical modelling strategy adopted here follow methodologies previously developed and validated and are therefore only briefly summarized [1, 2]. Figure 1 illustrates the geometry of the notched specimen along with its general dimensions.

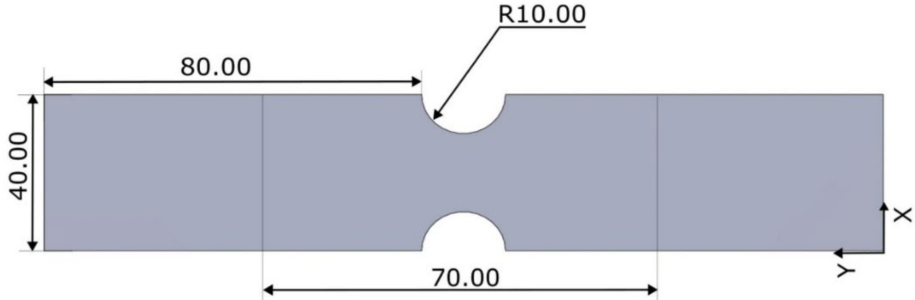


Fig. 1. Geometry of the notched specimen [1].

Full-field displacement and strain measurements are obtained experimentally using Digital Image Correlation (DIC). These measurements provide spatially resolved information over the specimen surface throughout the loading history and serve as the experimental reference data for the inverse identification procedure. The numerical simulations are performed using Abaqus under quasi-static conditions. The specimen is discretized using two-dimensional finite elements to accurately capture strain gradients and localization effects, while maintaining a reasonable computational cost. Experimentally measured displacement fields are prescribed as boundary conditions on the model, ensuring consistency between experimental and numerical loading paths.

A static general analysis step with automatic time incrementation is employed, using an initial increment of 10^{-3} and minimum and maximum allowable increments of 10^{-4} and 10^{-2}, respectively. These settings were selected based on previous numerical studies on heterogeneous specimens and were found to provide a robust compromise between numerical stability and computational efficiency. To enable a consistent comparison between experimental and numerical strain fields, experimental data are interpolated onto the finite element mesh. The interpolation and mapping strategy ensures spatial alignment between experimental measurement points and numerical integration points while accounting for differences in discretization and field resolution. As this framework has been previously developed and validated, further details are not repeated in the present work.

Surrogate-assisted Bayesian optimization

The calibration problem addressed in this work is formulated as an inverse identification task in which a set of constitutive parameters is determined by minimizing a cost function derived from the differences between experimental and numerical data. Each evaluation of the objective function requires a complete finite element simulation of the notched specimen tensile loading test, making the optimization process computationally expensive. As a result, the use of classical gradient-based or exhaustive search strategies becomes impractical. To mitigate this limitation, a surrogate-assisted Bayesian optimization framework is adopted.

Bayesian optimization is particularly suited for problems characterized by expensive, non-convex, and potentially noisy objective functions. In the present context, FEMU is treated as a black-box function that maps a vector of material parameters to a scalar cost function value derived from full-field strain discrepancies.

Material behavior and parameter space.

The material behaviour is described using an elastoplastic constitutive model with isotropic hardening. Elastic deformation is modelled by linear isotropic elasticity according to Hooke's law, while plastic yielding is governed by a von Mises equivalent stress criterion. The yield function is expressed as

$$f(\boldsymbol{\sigma}, \overline{\varepsilon^{\mathrm{p}}}) = \bar{\sigma}(\boldsymbol{\sigma}) - \sigma_{\mathrm{y}}(\overline{\varepsilon^{\mathrm{p}}}), \quad (1)$$

where $\bar{\sigma}(\boldsymbol{\sigma})$ stands for the equivalent stress defined based on the Cauchy stress tensor $\boldsymbol{\sigma}$. The evolution of the flow stress, σ_{y}, defined as a function of the equivalent plastic strain, $\overline{\varepsilon^{\mathrm{p}}}$, is described according to the Swift hardening law as

$$\sigma_{\mathrm{y}}(\overline{\varepsilon^{\mathrm{p}}}) = K\ (\varepsilon_0 + \overline{\varepsilon^{\mathrm{p}}})^n\ , \quad (2)$$

where the nonlinear isotropic hardening behaviour is fully characterized by the parameter vector θ,

$$\theta = [K, \varepsilon_0, n], \quad (3)$$

that defines the search space explored in the inverse identification procedure. Parameter bounds are selected based on prior calibration studies and physically admissible ranges, ensuring stable numerical simulations and meaningful material responses throughout the optimization process.

FEMU cost-function based on full-field data.

For a given parameter vector θ, a finite element simulation of the notched specimen test is performed and numerical strain fields are obtained. These fields are compared to experimentally measured strain fields acquired by Digital Image Correlation (DIC). After interpolation schemes, the discrepancy between experimental and simulated results with the θ vector of material parameters is condensed into a scalar cost function defined as

$$CF(\theta) = \frac{1}{n_t}\sum_{i=1}^{n_t}\left\{\frac{1}{3n_p}\sum_{j=1}^{n_p}\left[\left(\frac{\varepsilon_{xx}^{\mathrm{num}}(\theta)-\varepsilon_{xx}^{\mathrm{exp}}}{\varepsilon_{\mathrm{xx,max}}^{\mathrm{exp}}}\right)^2+\left(\frac{\varepsilon_{yy}^{\mathrm{num}}(\theta)-\varepsilon_{yy}^{\mathrm{exp}}}{\varepsilon_{\mathrm{yy,max}}^{\mathrm{exp}}}\right)^2+\left(\frac{\varepsilon_{xy}^{\mathrm{num}}(\theta)-\varepsilon_{xy}^{\mathrm{exp}}}{\varepsilon_{\mathrm{xy,max}}^{\mathrm{exp}}}\right)^2\right]_j+\left(\frac{F^{\mathrm{num}}(\theta)-F^{\mathrm{exp}}}{F_{\mathrm{max}}^{\mathrm{exp}}}\right)^2\right\}_i \quad (4)$$

where F^{exp} corresponds to the grips' reaction force that was recorded using a load cell. Regarding the strain components $\varepsilon_{\mathrm{xx}}$, $\varepsilon_{\mathrm{yy}}$, and $\varepsilon_{\mathrm{xy}}$, these are computed based on the displacement fields, both numerical and experimental, by the identification software. To enable a straightforward comparison of these quantities, the experimental displacements at the DIC points were interpolated to the FE nodes. The superscripts num and exp refer to the data iteratively generated along the numerical optimization process and to the experimental data, respectively. n_{t} is the number of time instances decided to be used by the authors and n_{p} is the number of measured points. $F_{\mathrm{max}}^{\mathrm{exp}}$ refers to the maximum load value achieved by the test and $\varepsilon_{\mathrm{max}}^{\mathrm{exp}}$ to the maximum strain value of the given strain component. This formulation enables the use of full-field information while yielding a single scalar objective suitable for surrogate-based optimization.

Bayesian optimization strategy.

Bayesian optimization proceeds by constructing a probabilistic surrogate model that approximates the relationship between the parameter vector θ and the FEMU cost function ϕ. In this study, a Gaussian Process (GP) regression model is employed due to its flexibility and its ability to provide both a mean prediction and an associated uncertainty estimate.

Starting from an initial dataset composed of a limited number of FEMU evaluations (five initial simulations), selected using Latin hypercube sampling (LHS) within empirically defined parameter ranges, due to its near-random design and efficient space-filling properties, the Gaussian Process (GP) surrogate is iteratively updated as new data become available. At each iteration, the surrogate model is conditioned on all previously evaluated parameter sets and their corresponding cost function values, yielding a predictive mean, μ, and standard variation, s, over the parameter space. An acquisition function is then maximized to identify the most informative next parameter set to evaluate, which is subsequently assessed through a new FEMU simulation and added to the training dataset.

In this work, the Expected Improvement (EI) criterion is adopted, defined for the minimization problem as

$$\mathrm{EI}(\theta) = \big(CF_{\mathrm{best}} - \mu(\theta)\big)\Phi(Z) + s(\theta)\phi(Z) \quad (5)$$

with

$$Z = \frac{CF_{\mathrm{best}}-\mu(\theta)}{s(\theta)} \quad (6)$$

where CF_{best} denotes the lowest cost function value observed so far and $\Phi(\cdot)$ and $\phi(\cdot)$ are the cumulative distribution function and probability density function of the standard normal distribution, respectively. This acquisition function naturally balances exploration of regions associated with high predictive uncertainty and exploitation of regions expected to yield lower cost function values.
The overall optimization loop is schematically summarized in Figure 2 and can be described as follows:

1. Fit the GP surrogate model to the current dataset of evaluated parameter sets and cost function values.
2. Minimize the acquisition function to select a new candidate parameter vector, θ_{new}.
3. Perform a FEMU evaluation for the selected parameters set(s), including finite element simulation and cost function computation.

4. Augment the dataset with the new evaluation and repeat the process for the selected number of trials.

Each evaluation of the FEMU cost function requires a full finite element analysis. For a given parameter vector θ, the constitutive law parameters are updated in the finite element model, and a numerical simulation is performed to compute displacement and strain fields. These numerical fields are then compared to the corresponding experimental full-field measurements, and the discrepancy is quantified through the FEMU cost function, $CF(\theta)$. Due to the high computational cost associated with each finite element evaluation, Bayesian optimization is employed to efficiently guide the selection of new parameter sets.

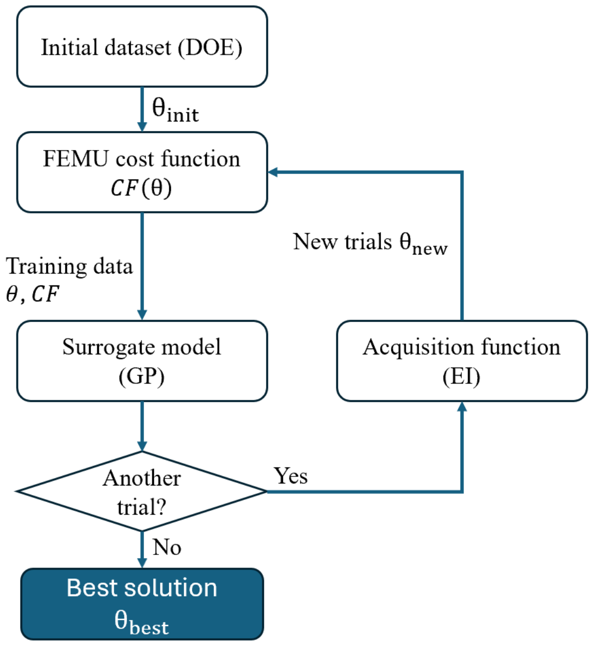


Fig. 2. Workflow of the Bayesian optimization procedure. Each evaluation of the cost function involves a finite element simulation to compute numerical displacement and strain fields, which are compared with experimental full-field data. Adapted from [12].

Results and Discussion

This section presents the results obtained with the proposed surrogate-assisted Bayesian optimization framework applied to FEMU calibration from a single notched specimen tensile loading test. As the present contribution is intended as an exploratory study, the discussion focuses on convergence behaviour, optimization efficiency, and qualitative assessment of the identified material parameters rather than on exhaustive parametric validation.

Optimization behaviour and parameter space exploration.

Figure 3 illustrates the evolution of the FEMU cost function during the Bayesian optimization process, together with the best-so-far value obtained after each trial. It is worth noting that the parameter set and, consequently the CF value, of the first trial is highly dependent on the samples composing the initial dataset. The existence of a sample in the initial dataset that already presented a significant low CF value influenced the optimization problem behavior. As the optimization progresses, the balance between exploration and exploitation allows the algorithm to explore regions of the parameter space associated with higher CF and, at the same time, to refine the solution, ultimately leading to a stable best-so-far value and practical convergence within a limited number of FEMU evaluations (16). It should be noted that the CF value could have achieved lower values if more trials were chosen.

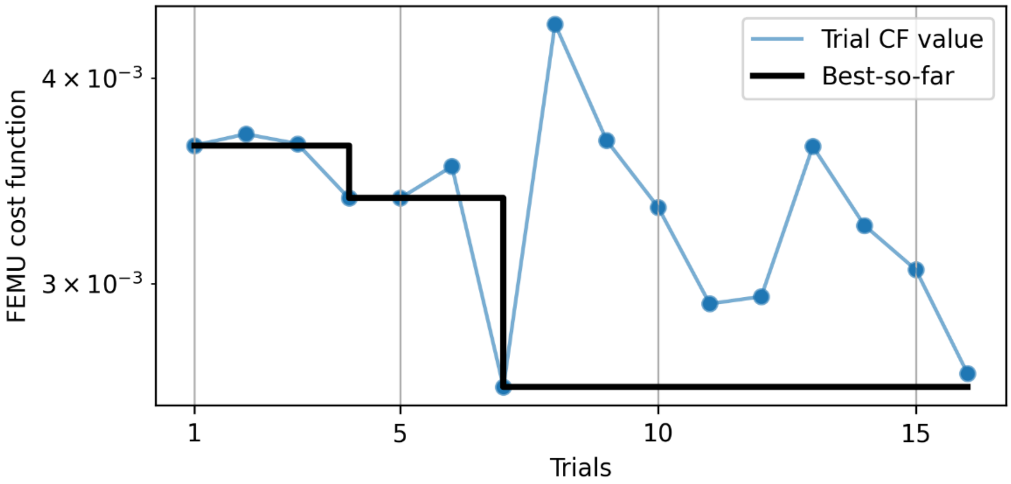


Fig. 3. Evolution of the FEMU cost function, *CF*, as a function of the number of trials. Individual markers represent the cost function values obtained at each FEMU evaluation (BO trial), while the best-so-far curve highlights the convergence behaviour of the optimization process.

To further analyse the behaviour of the Bayesian optimization procedure, the distribution of the parameter sets in the design space is examined. Figure 4 illustrates the projection of the sampled points onto selected two-dimensional parameter subspaces, allowing the exploration strategy of the algorithm and the location of the identified optimal solutions to be visually assessed.

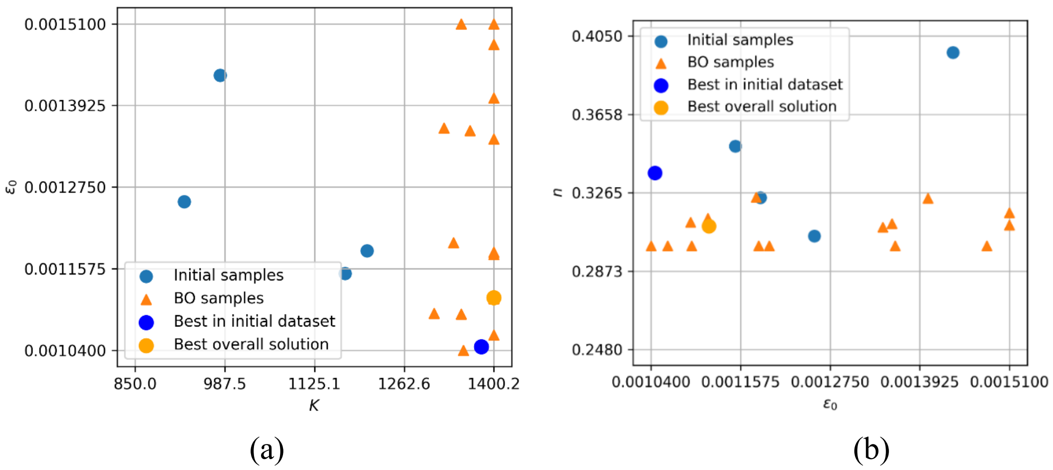
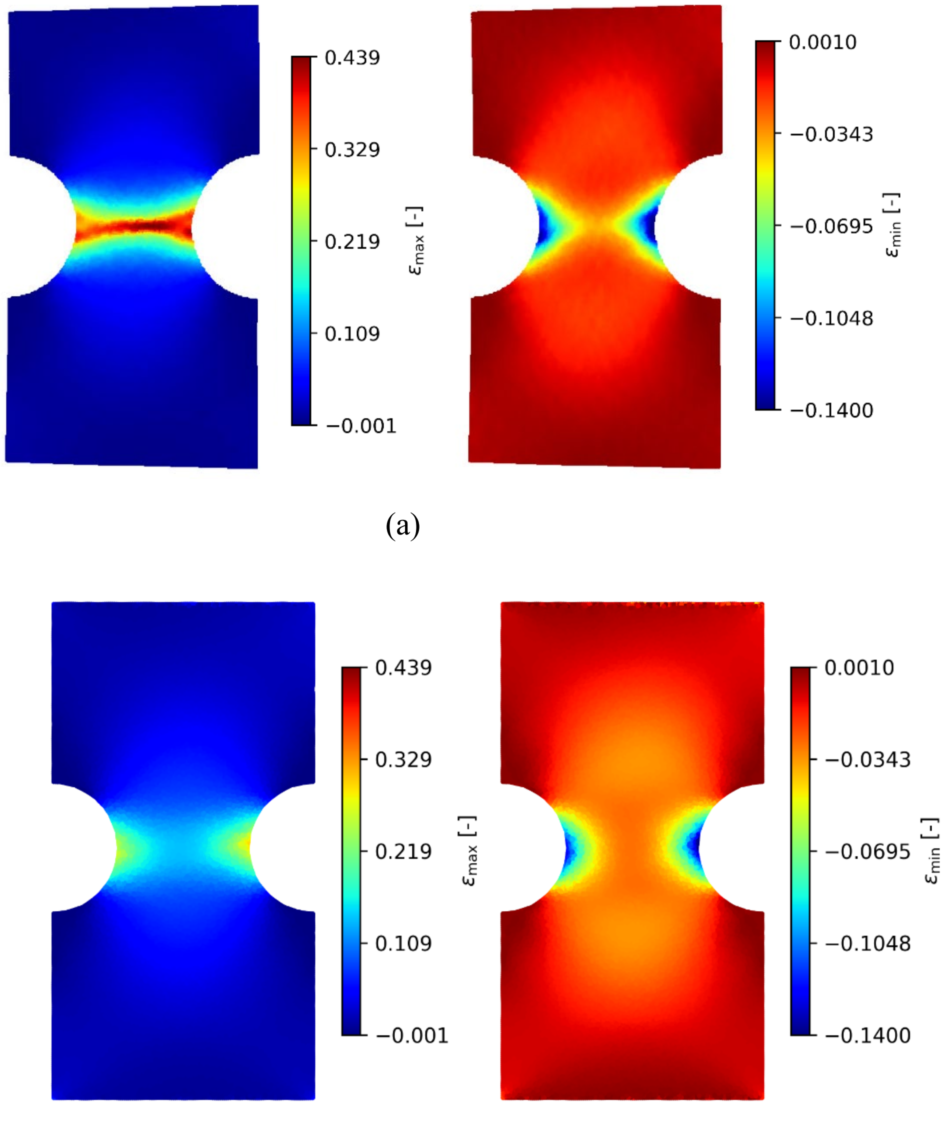


Fig. 4. Samples distribution in the parameter space projected onto selected two-dimensional planes: (a) K–ε_0 and (b) ε_0–n. Initial samples are shown in blue, BO-generated samples in orange, together with the best parameter set from the initial dataset and the overall best solution identified during the optimization.

The initial samples (blue dots) correspond to the five evaluations presented in the initial dataset, which parameter sets were generated by LHS method. Based on these data, the BO method, specifically the acquisition function, decide which parameter set to try next (trial). At each trial, a BO sample is generated, corresponding to the orange triangles (cf. Figure 4). After 16 trials, the optimization ends with the best solution so-far in the process. This one as well as best solution presented in the initial dataset are highlighted in the same colour of the group which are a part of, BO samples and initial dataset, respectively. The distribution of the BO-generated samples indicates an initial exploratory phase covering a broader region of the parameter space, followed by a progressive concentration of samples around regions associated with lower cost function values. These results indicate the possibility that the optimisation procedure became trapped in a local minimum. Increasing the dimensionality and diversity of the initial dataset or evaluating other options for the acquisition function could improve the search capability to avoid premature convergence.

Identified parameters and full-field agreement.

Figure 5 presents a comparison between experimental and numerical strain fields obtained using the best set of material parameters identified through the methodology presented in this work. The experimental strain maps are derived from full-field measurements, while the numerical strain fields are computed from finite element simulations using the calibrated constitutive model.



(b)

Fig. 5. Comparison between the (a) experimental and (b) numerical strain fields for the notched specimen tensile specimen using the set of parameters corresponding to the best solution of the Bayesian optimization approach.

The material parameter set identified as the best solution at the end of the Bayesian optimization process is found to be physically plausible and consistent with reference values reported in previous calibration studies. The corresponding numerical results reproduce the main features observed experimentally, including strain localization patterns and gradients in the notch region. These qualitative observations confirm that the reduction in the FEMU cost function achieved during optimization corresponds to a good improvement in the reproduction of experimentally observed deformation mechanisms. Nevertheless, a perfect agreement between experimental and numerical strain fields is not achieved. This indicates that the parameter set identified as optimal with respect to the adopted cost function does not necessarily correspond to the true physical material parameters. Such discrepancies may stem from multiple sources, including limitations of the inverse identification procedure, experimental uncertainties, chosen test specimen or constitutive model. Moreover, this observation must be interpreted in light of the intrinsic non-uniqueness of inverse problems, where different parameter combinations may lead to similarly low-cost function values and comparable full-field responses. In addition, the robustness of the optimisation framework itself may influence the outcome, as the final solution remains dependent on the initial dataset, the dimensionality of the sampled space, and the balance between exploitation and exploration governed by the acquisition function. Insufficient global search capability may prevent convergence towards the true global optimum.

Conclusion

This work presented an exploratory investigation of surrogate-assisted Bayesian optimization for FEMU-based material model calibration using full-field strain data obtained from a single heterogeneous notched tensile test. The proposed framework couples FEMU with a probabilistic surrogate model to efficiently explore the material parameter space while limiting the number of computationally expensive finite element simulations.

The observed convergence behaviour indicates that Bayesian optimization can effectively guide the calibration process. The main strength of the proposed approach lies in its ability to efficiently explore parameter space and to identify promising regions using a limited number of costly finite element evaluations. In this sense, Bayesian optimization provides a suitable data-driven layer on top of full-field FEMU, offering a flexible and computationally more efficient alternative to traditional gradient-based or exhaustive search strategies.

Nevertheless, several limitations must be acknowledged. The present study is intentionally restricted to a single heterogeneous test and a limited parameter space, and no systematic investigation was conducted on the influence of different acquisition functions, the size of the initial training dataset, or the number of optimization trials. The use of other acquisition functions which allow setting hyperparameters regarding the exploration-exploitation balance may improve the search in the parameter space, avoiding being trapped in a local minimum.

Despite these limitations, the proposed methodology constitutes a solid and extensible basis for future developments. Further work will focus on extending the approach to more complex heterogeneous tests and constitutive models, as well as on systematically investigating the influence of initial sampling strategies, surrogate model hyperparameters, and acquisition function choices. Such studies will be essential to fully assess the robustness, reliability, and general applicability of Bayesian optimization–assisted FEMU for material parameter inverse identification.

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