NEW OPPORTUNITIES AND BENEFITS IN THE PRODUCT DEVELOPMENT PROCESS USING THE MACHINE LEARNING BASED DIRECT INVERSE METHOD FOR MATERIAL PARAMETER IDENTIFICATION

Meißner, Paul;
Vietor, Thomas

Institute for Engineering Design, Technische Universität Braunschweig

ABSTRACT

Finite element (FE) simulations can be used both in the early product development phase to evaluate the performance of developed components as well as in later stages to verify the reliability of functions and components that would otherwise require a large number of physical prototype tests. This requires calibrated material cards that are capable of realistically representing the specific material behavior. The necessary material parameter identification process is usually time-consuming and resource-intensive, which is why the direct inverse method based on machine learning has recently become increasingly popular. Within the neural network (NN) the generated domain knowledge can be stored and retrieved within milliseconds, which is why this method is time and resource-efficient. This research paper describes advantages and potentials of the direct inverse method in the context of the product development process (PDP). Additionally, arising transformation opportunities of the PDP are discussed and an application scenario of the method is presented followed by possible linkage potentials with existing development methods such as shape optimization.

Keywords: Machine learning, Material parameter identification, Simulation, Neural Networks, Computational design methods

Contact:
Meißner, Paul
TU Braunschweig
Germany
p.meissner@tu-braunschweig.de

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1 INTRODUCTION

Companies are constantly striving to shorten product development times in order to meet the increasing product requirements on the market and to succeed in competition. The time-to-market is a decisive factor for the success of a new product (Afonso et al., 2008). This pressure of time further intensifies due to the significant increase in demand for customized products and the growing number of different product variants in recent years (Schuh et al., 2019). This leads to a more complex design phase, as the specific material properties have to be considered and ideally utilized in the design and different materials may require different design variants. Simultaneously, the demand for the remaining or even increasing product quality exists. For example, in automotive engineering vehicle safety regulations (N.H.T.S.A., 2008; Euro-NCAP, 2020) and emission requirements (Elgowainy et al., 2018; Kim et al., 2011) are continuously increasing, leading to a more challenging product development process (PDP).

Faster product development is usually coupled with cost reductions, but it also involves the risk of insufficient production readiness, which in turn is associated with recall and re-development costs (Albers and Nowicki, 2003). A larger number of iterations during product development, e.g. due to the non-fulfillment of specified requirements and the associated necessary repetitions of specific development steps, has negative effects on the development costs as well as on the development time. Therefore, the use of computer-aided engineering (CAE) tools is indispensable nowadays and is applied throughout the entire PDP. Finite element (FE) simulations are used, for instance, both in early phases to evaluate the performance of developed components before manufacturing and production and also in later phases to ensure the safety and function of components or the entire product (Kohar et al., 2021). This allows reducing the amount of necessary physical prototypes and the associated time- and cost-intensive development iterations, as well as allowing the design engineers to gain a better understanding of component and assembly features. Additionally, it is possible to define relevant design parameters and performing parameter studies on the virtual prototype to fulfill the desired product requirements.

A crucial input of the FE analysis (FEA) is the material model, which describes together with the material parameters (MP) the constitutive relationship of the induced stresses as a function of the applied loads and thus represents the real material behavior (Jones et al., 2018). Often these MP have no direct physical meaning and cannot be determined directly from experimental studies. Even in physically inspired material models, the MP are fitable model parameters utilized in order to approximate the real material behavior in conjunction with the material model. Consequently, the MP must be calibrated in a material parameter identification (MPI) process to achieve the highest possible agreement between simulation and reality (Mahnken, 2018). Thus, the calibrated material model has a significant influence on the resulting accuracy and validity of the FEA.

Apart from the rather rudimentary manual trial and error process, there are two basic and one hybrid method for MPI, for which no uniform definition of the name or the specific process steps exists (see Figure 1). In the **iterative optimization-based method**, numerical simulations are performed on the basis of a sampled set of material parameters, and a specific error measure (e.g. mean squared error of load-displacement curves) is calculated between these and the experimental results (Mahnken, 2018). Then, this error is minimized in an iterative process using appropriate optimization algorithms by modification of the MP. The process ends when a certain termination criterion such as a specific precision criterion or a maximum number of iterations is reached. However, this method requires a high degree of expert knowledge and for complex material models typically numerous iterations with accompanying high computational costs are necessary. Also, the suitability of the MP significantly depends on the choice of starting parameters and parameter bounds (Morand and Helm, 2019).

In an alternative **hybrid ML-based approach**, ML algorithms such as neural networks (NN) are used to replace time-intensive numerical simulation and predict the results in the form of load-displacement curves, for instance (Aguir et al., 2011). In a subsequent optimization, the MP can be iteratively adjusted for a higher agreement between experiment and simulation.

Contrary to the hybrid method, in which the input data are material parameters and the output are resulting curves, the relationship of the **direct inverse MPI method** is exactly reversed. In this case, a surrogate model (e.g. a neural network) is taught the relation between numerical simulation results and the corresponding MP so that in the application step experimental test curves can be imported into the surrogate model and suitable MP can be predicted (Unger and Könke, 2011). No subsequent optimization is performed, since the training of the NN represents the optimization, whereby in contrast

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to the **conventional** or **hybrid** method not the error measure of the result curves but a special loss function (e.g. MSE) of the MP is minimized. This is both an advantage and a disadvantage since although the minimization is not performed on the actual objective of the MPI method, no time-intensive FE simulations are necessary either. Thus, the method is resource efficient, especially when used repeatedly, since the generated knowledge can be stored in the NN and retrieved within milliseconds.
Due to the increasing number of used materials with complex material behavior (such as polymers) as well as the ambition to implement FEA in the product development process, there is a high demand for MP calibrations. Due to the required comprehensive expert knowledge, necessary computational resources and time-consuming calculations as well as complex experimental investigations, these represent a hurdle for implementing FEA more extensively as well as earlier in the PDP. Small and medium-sized companies often do not have the in-depth expertise regarding continuum mechanics, material parameter identification, and optimization processes or the appropriate resources to integrate the necessary efforts into their PDP. Hence, this article will highlight the advantages and potentials of the **direct inverse method** for product development, as well as present how this method can be applied in the PDP and potentially transform it. In this context, the potentials of direct inverse MPI in relation with the further increasing importance of recyclate use are also addressed. Furthermore, existing research demands as well as linking opportunities with methods of computer-aided design are revealed.

2 STATE OF THE ART AND RESEARCH

In the following, the basics for understanding the advantages and potentials of direct inverse MPI as well as its integration into the product development process are briefly presented.

2.1 Material parameter identification

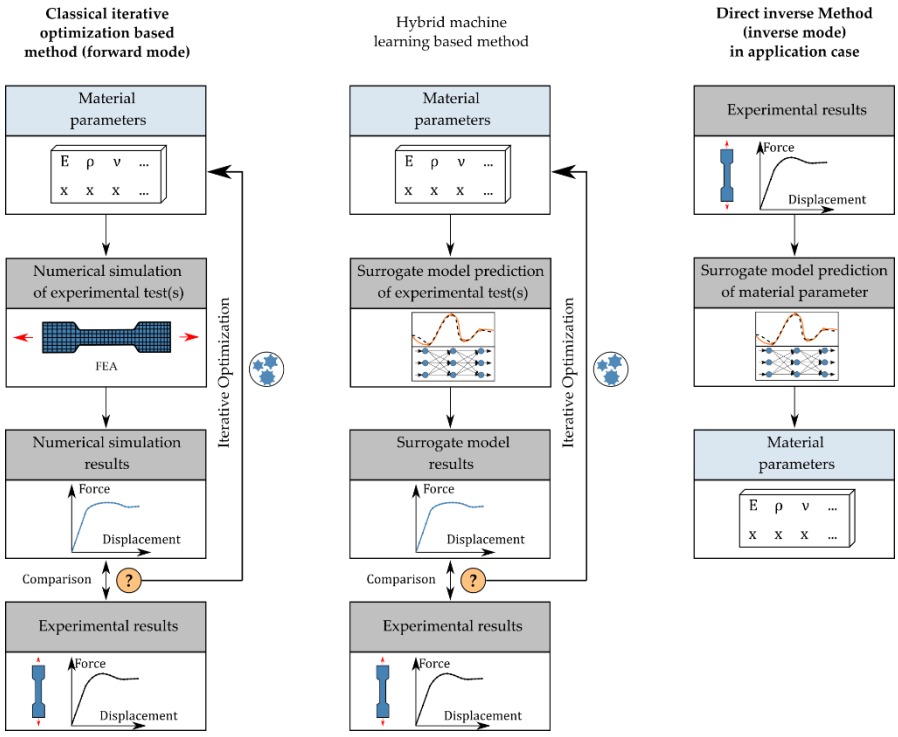

Figure 1. Methods for material parameter identification

Besides the trial and error approach, the MPI process comprises solving an inverse (identification) problem to identify or estimate the system parameters from the measured system response (Stavroulakis et al., 2003). This process does not have consistent terminology and is often referred to as calibration of a material card, which is the input for the software implementation of a material model in a special FE solver. However, this requires the fundamental capability of the material model to reproduce the underlying material characteristics. Two main methods are distinguished to solve this identification problem. In the **iterative optimization-based method** described by Kučerová (2007) as **forward (classical) mode**, an error function is defined as the difference between parameterized model

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outputs and experimental measurements, which is usually minimized using an optimization algorithm (e.g. gradient-based or genetic algorithm). Often difficult highly nonlinear and multi-modal optimization problems result from this. In order to reduce the extensive computational costs, meta-models usually are applied, whereby sometimes NNs are used as surrogate models. For the application of the iterative optimization-based method commercial software solutions like LS-OPT exist, but also in-house developed software is often. As mentioned in Section 1, the **hybrid MPI approach** is based on the forward mode, whereas the time-consuming FE simulations are replaced by the usage of a surrogate model, e.g. an NN (Aguir et al., 2011). The main advantage of this approach is the reduction of necessary CPU time compared to the classical inverse method.
In the second main method, the **direct inverse method**, which is also called inverse mode by Kučerová (2007), the existence of an inverse relationship between output and input is assumed and the material model is effectively inverted using a surrogate model. The surrogate model (e.g. NN) is trained using simulated material responses from the FEA as input and directly predicts the model parameters. This method is presented in more detail below. The three approaches for MPI are compared in Figure 1.

2.2 Direct inverse material parameter identification method

Similar to the classical forward mode, there is no standardized procedure for the direct inverse approach. In the following, it will be described most generally, referring to the specific implementation of (Meißner et al., 2022a) as an example (see Figure 2).

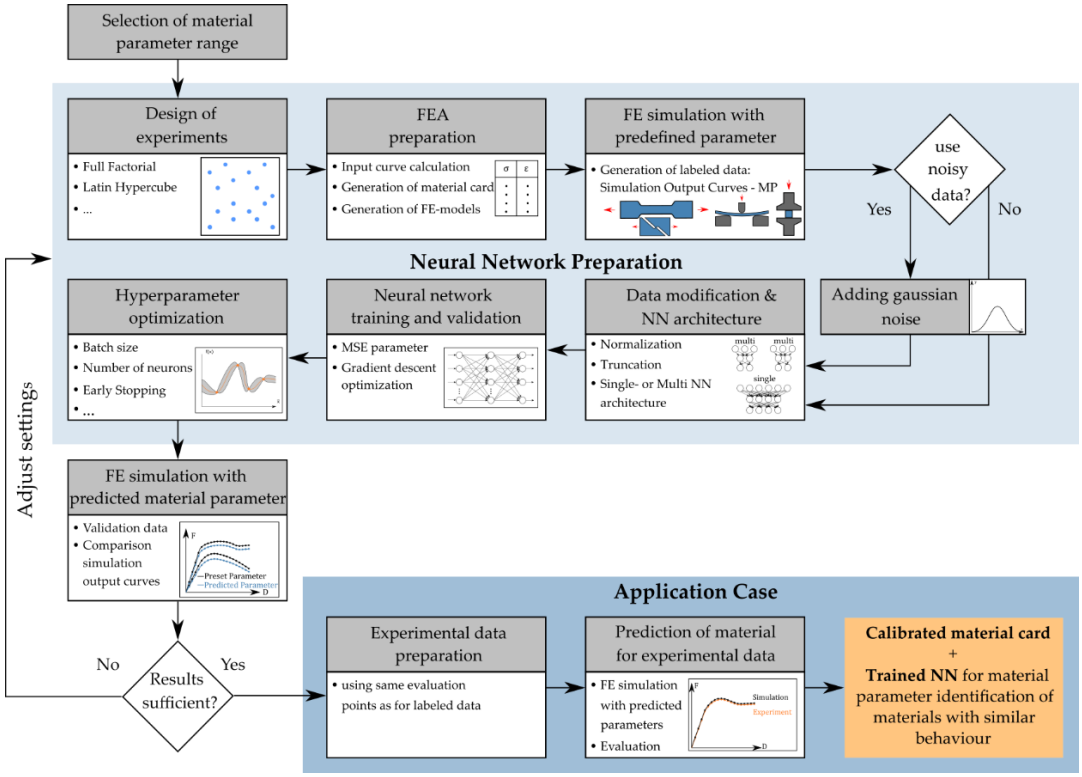

Figure 2. Flow chart of direct inverse material parameter identification method, implementation and illustration of (Meißner et al., 2022a)

Analogously to the forward mode, initially a material parameter range is selected that is assumed to contain the solution of the inverse problem. Using appropriate sampling methods, MP sets (system parameters) are defined in a design of experiments (DOE) and subsequently, multiple numerical simulations are performed. The results of the simulation are usually time series (e.g. load-displacement curves). In recent years it has been demonstrated that data augmentation strategies like random transformations in time series tasks are often suitable for increasing the prediction accuracy (Demir et al., 2021). Hence, it can be advantageous to apply data augmentation methods in addition to basic data modification such as normalization and truncation. This includes, for example, the application of a Gaussian noise, which also improves the generalization capability of the NN and thus its performance

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on unknown data. Furthermore, the methodology is not limited to NNs or an NN type as a surrogate model, although in the past mostly multilayered perceptrons were used. During training, the NN learns the relationship of the labeled data. The loss function is usually based on a distance measure of the different MP. Since hyperparameters like the number of neurons in the respective layers, the batch size or other architecture determining parameters have a large influence on the prediction accuracy, a hyperparameter optimization is often performed to increase the performance of the approach. Subsequently, using the predicted MP, numerical simulations are again executed. Typically, this is done on a validation dataset to verify the performance of the prediction for the overall aim of the method, which is the match of the simulation results with the predefined data. If this accuracy is not sufficient, previous steps can be repeated and additional input data can be generated or settings can be adjusted. Finally, the target is to import the experimental measurements and directly predict the MP which are suitable for reproducing the material behavior in the numerical simulation sufficiently precisely. Since the knowledge is stored in the parameters of the NN, the final prediction can be repeated in milliseconds for other experimental datasets. Prerequisites for a constant prediction accuracy are the fundamental suitability of the reproduction with respect to the material characteristics to be described as well as the sufficient coverage of the parameter range of the new measurement dataset.

The method was first introduced by Yagawa et al. (1996) to determine parameters of a viscoplastic material model and since then this approach has been applied to various materials. Chamekh et al. (2009) demonstrated that using suitable ANNs, this direct inverse approach can also identify MPs to describe anisotropies by determining the anisotropic HILL parameters of an elasto-plastic model. Mareš et al. (2016) investigated different strategies for calibrating nonlinear models using NN. However, they achieved comparatively poor results using the direct inverse MPI method. They explained this with the not necessarily existing inverse relationship and the challenge to approximate it as well as the high sensitivity of the NN to experimental measurement errors. Meißner et al. (2022b) compared the resulting prediction accuracy using the different network types Multilayer Perceptrons (MLP), Convolutional Neural Networks (CNN) and Bayesian Neural Networks (BNN) and investigated different network architectures and topologies. They demonstrated their applicability for the complex material card MAT_187_SAMP-1 of the solver LS-DYNA for the simulation of thermoplastics and achieved the highest prediction accuracy with CNNs.

3 DIRECT INVERSE MATERIAL PARAMETER IDENTIFICATION METHOD IN PRODUCT DEVELOPMENT PROCESS

3.1 Material cards in product development

The importance of FEA and material cards is explained below using the V-model in product development, which is based on VDI 2226 (Technical Commitee 4.10, 2022), see Figure 3.

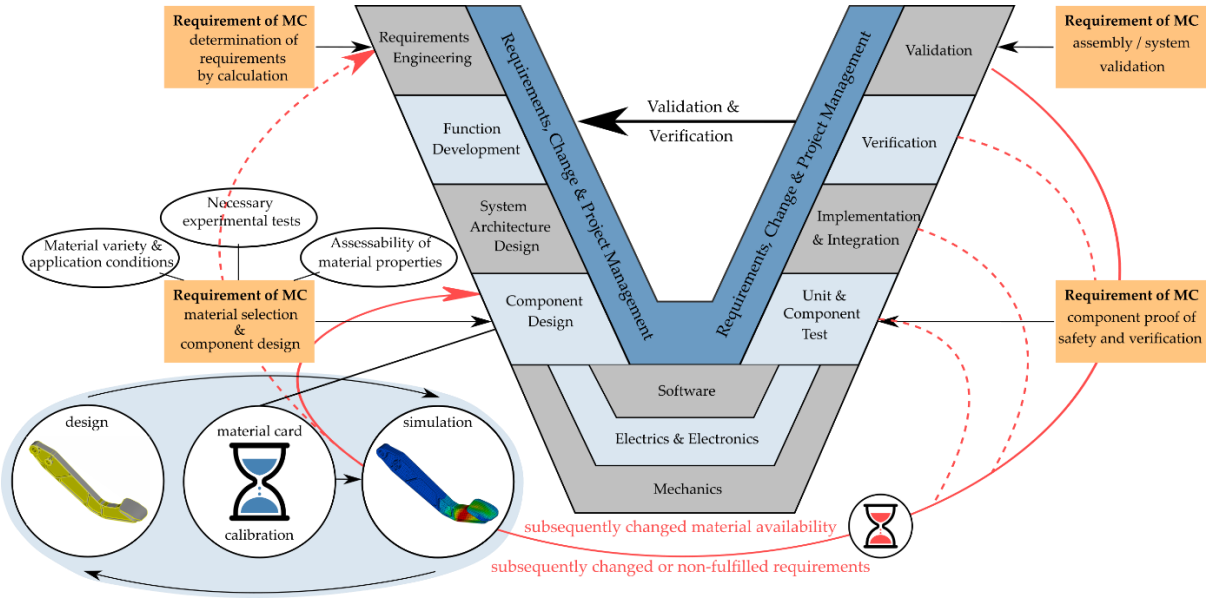

Figure 3. Requirement of material cards in V-model of product development process

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Here, the left leg of the V represents the decomposition of the system into its elements, and the opposite side on the right stands for the integration of elements and subsystems into the overall system. Constant verification and validation of the properties of the system under development takes place in between, which is associated with requirements, change and project management.
Already when determining the requirements for the product, the first FEAs can be used to evaluate the occurring loads and the resulting stresses according to load paths. These calculations help development engineers for a better understanding of the effective mechanisms. The more precisely the requirements can be determined, the more accurately a product can be developed and adapted to fulfill them. Also, the corresponding effort and costs can be estimated. Consequently, this reduces the risk of oversizing and failure of the product in verification and validation tests during the remaining development process, which would result in increased workload and costs due to rework. Often, at this development stage, the materials to be used have not yet been defined and a detailed material card is usually not yet available. Nevertheless, it is possible to make engineering assumptions regarding stiffness and strength, neglecting specific material characteristics and still perform various calculations to determine requirements. However, the more precise calculations can be carried out at this early stage, the smaller will be the gap between determined and actual product requirements.
A major use of FEA in PDP comes during the component design phase. Here, the component has to be designed appropriately to withstand external loads. Component properties such as deformations, energy absorption, acoustic properties, etc. have to be analyzed and the component structure has to be dimensioned accordingly, e.g. by adjusting component body thicknesses. Especially when working with complex materials such as polymers or fiber-reinforced composites, it is essential to consider the specific material properties. Often, there is a multitude of possible materials with diverging mechanical properties such as stiffness, failure strain, softening temperature, etc. Material data sheets are often used for this purpose, but they only provide a first impression of the specific material behavior and do not represent the complete material characteristics. This includes characteristics such as failure strains at a specific stress state or energy absorption until failure as well as material characteristics such as hardening and softening. Additionally, their effect on the component performance is difficult to evaluate. Such information is time-consuming and cost-intensive to determine since often complex experimental investigations are required. However, the choice of material is also influenced by economic and ecological properties such as price, availability, CO_2 footprint, etc. Based on these aspects, which are sometimes difficult to quantify, one or more potential materials are usually selected for the design process. In a commonly iterative process, an initial design is created by the engineer and the fulfillment of defined requirements is verified in an FEA. Occasionally, some materials require different design concepts, which further increases the complexity of the design process. If the requirements are not or only partially fulfilled, the design must be re-adapted in an iterative process and subsequently checked in the calculation. Often, design optimization strategies such as topology optimization (TPO) are used for this task. Although, e.g. for crash-loaded components, this requires precise nonlinear numerical simulations considering the specific material behavior, which is why material cards are needed for this product development stage. If these are not available for the materials to be potentially used, they must be determined in an MPI process. If the complexity exceeds simple material characteristics, an iterative optimization-based MPI is usually performed for each potential material. Due to the high computational effort, this slows down the further progression of the PDP.
Following, tests are conducted to verify the fulfillment of the specified requirements and to ensure product safety. In this development phase, FEA contributes to acceleration and cost reduction, since the number of necessary prototypes and cost-intensive experimental tests can be drastically reduced through the use of numerical simulations. The prerequisite for this is once more highly precise simulations, with which a detailed representation of reality is possible. If the requirements are not met, development steps have to be repeated, which increases costs and development time. From a materials engineering point of view, for example this can occur if the material does not meet the minimum specifications or exhibits too much variation, or if the material availability and similar factors have changed. Unless it is possible to switch to an alternative material and consequently a new material must be selected, the development process may significantly delay due to the MPI process being conducted again. This also applies, if in the final stage the requirements are not met when the entire assembly or system is validated. Hence, the need to calibrate material cards as quickly as possible can arise several times within the PDP.

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3.2 Application scenario and transformation opportunities through direct inverse MPI

The previously described extract of the usage of material cards in the PDP highlights the benefits of direct inverse MPI. In the following, an application scenario is presented to demonstrate the advantages and potential savings when using this method (see Figure 4). This scenario is initially focused on the *component design* development step (see Figure 3) and following more potentials are discussed.

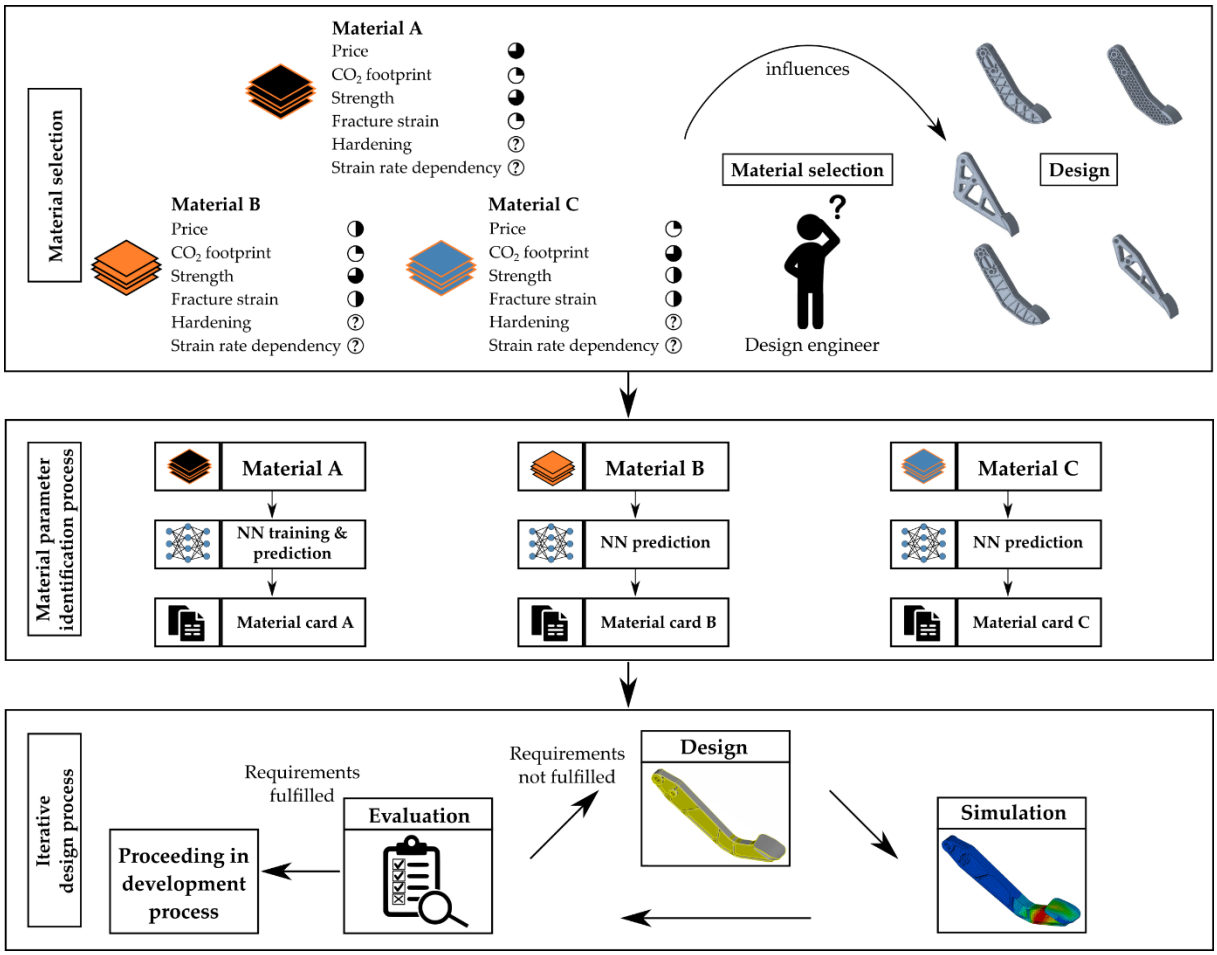

Figure 4. Application example of the direct inverse material parameter identification method in the component design development step in PDP

Initially, different materials with divergent properties are available to the development or design engineer in order to develop a component that fulfills the previously defined requirements. In this scenario, it is previously assumed that a thermoplastic material should be used, thus the underlying material characteristics of the possible applicable materials are similar. Some of the material properties and attributes, such as its price, can be quantified directly, while for other properties, such as material characteristics like hardening and strain rate dependency, both the characteristics and their impact on product performance cannot be determined directly from a product data sheet and are difficult to estimate. Additionally, some materials may benefit from different design approaches. To compare different designs and to dimension the component appropriately, numerical simulations and consequently material cards are required. Using direct inverse MPI, numerical simulations generate labeled data for a defined range of MP, allowing an NN to be trained, and to predict the MP required for FEA on experimental test data. For the alternatively available materials, this NN can now be reused without repeated simulation efforts or training, and appropriate MP can be predicted in milliseconds. Consequently, the design drafts can now be evaluated in FEA and compared with each other, depending on the materials used. In the following iterative simulation-based design process, the designs are optimized, which drastically reduces the probability of subsequent failure to fulfill the requirements in unit or component tests. By using the direct inverse MPI approach compared to the conventional forward method, valuable development time could be saved.

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Besides this scenario, there are other directly or indirectly related advantages and potentials. For instance, if pre-trained NN or other surrogate models can be used at the beginning of the PDP to define requirements and thus generate precise material cards early on, it is possible to define very precise requirements with the help of FEA. Thus, the risk of over- or undersizing can be reduced in the further PDP. If development steps have to be repeated and alternative materials have to be used for the development due to various influences in the PDP, the direct inverse MPI method can contribute to reducing additional time expenditures due to the reusability of the surrogate model (see Section 3.1). Whether the accuracy of the direct inverse approach is generally higher than that of the conventional or hybrid method cannot simply be evaluated, since the various settings and process steps that can be used make it difficult to carry out an adequate comparison, which is always related to the specific application. Furthermore, the direct inverse method is currently still a subject of research and many new methods in adjacent research areas still offer potential for improvement. However, if a highly precise simulation model with a detailed material card shall be built, it is possible to predict MP using the direct inverse method. Subsequently, these parameters can be used as starting parameters for the iterative optimization-based (forward) method. Since this method often tends to determine local minima, this procedure could provide an accuracy advantage or at least reduce the number of necessary iterations of the conventional method. This would be an advantage, especially on the right side of the V-model (see Figure 3), where various verifications and validations of requirement fulfillment are performed and high-precision simulations for safety assessment are often conducted.

Nevertheless, the scenario presented initially required the resource-intensive generation of labeled data using numerical simulations for a selected material. This is not necessarily more resource intensive than performing calibrations using the optimization-based forward method, but the direct inverse method offers the potential for further reduction. For example, pre-trained NNs could be provided by FE software companies or even material suppliers to allow users to directly generate appropriate material cards for subsequent FEAs without extensive calibration tasks. This represents a further advantage since no extensive expert knowledge in continuum mechanics, materials engineering, numerical optimization, etc. is required. This know-how often does not exist in small and medium-sized companies, which therefore represents a hurdle to the use of FEA in the PDP. If suitable pre-trained NNs are provided, only the experimental data would have to be obtained and imported into the NN. Thus, the integration of the direct inverse method into the commercial engineering software chain could be an enabler to increase the utilization of FEA in product development.

Due to the time-efficient reuse of the surrogate models, it is possible to calibrate a much higher number of specific material cards than would be reasonable from an economic point of view using the conventional method. This could be important in the future, especially with the increasing use of sustainable materials and recyclates as part of resource reuse efforts. Material recyclates (especially polymer recyclates) often exhibit a high variance in properties due to e.g. material mixtures as well as thermal or mechanical processing influences (Jubinville et al., 2021) and different batches of the same material compound distinguish often considerably. Nevertheless, if corresponding experimental data are available, the direct inverse approach could be used to generate batch-dependent material cards without additional time-consuming and cost-intensive numerical calculations. This could contribute to a better evaluation of the effects of property deviations on the structural component performance. Further advantages would arise especially concerning additive manufacturing since therefore no additional tooling costs are required for different designs with varying component dimensions. Thus, individual part-specific component dimensioning with batch-dependent material cards in a closed-loop digital design process would be possible. Since this avoids that presumably low quality material batches are always waste, a further step towards resource-saving product development could be accomplished.

Another issue that gains further importance in this context is the uncertainty quantification in parameter identification tasks (Rappel et al., 2020). Knowing and being able to evaluate the effects of different uncertainty quantities on the subsequent development process is a major advantage for ensuring product quality and reliability. Although uncertainties can also be quantified with the conventional MPI method using e.g. Bayesian inference approaches, it has been shown that the use of BNN in combination with the direct inverse method offers several additional advantages (Unger and Könke, 2011; Jospin et al., 2022). Here, the output of the NN is not only a deterministic value (in this case one or multiple MP) but a probability density function, from which statistics such as the standard deviation can subsequently be calculated. A distinction can be made between aleatoric and epistemic uncertainties, which provides additional information and enables data-efficient training. Furthermore, BNNs can be applied to decrease

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the risk of overlearning and thus increase the generalization ability. The integration of the direct inverse method in combination with uncertainty quantification approaches thus offers the potential to better evaluate and assess FEA results in the PDP and to make more profound development decisions.

3.3 Linking opportunities and future research focus

Nowadays, topology and shape optimizations are often used for computer-aided design. These allow the design to be iteratively adapted to the requirements, e.g. special energy absorption or maximum deformation under restrictions such as minimum weight and thus reduce manual design loops. Possibly, the full potential of the direct inverse MPI method can only be exploited in combination with these automatized design methods. From the authors' point of view, shape optimization is especially promising in this context, since it can incorporate complex nonlinear material behavior using complex material cards. By connecting the methods, shape optimization would be applied, for example, in the *iterative design process* step in Figure 4. Designs could be determined for different materials and compared based on specific criteria such as specific (density-related) mechanical properties. This would represent an important decision criterion in the material selection process for subsequent component manufacturing and production, enabling the right material to be selected for the respective application.

Furthermore, a reduction of the required experimental tests as surrogate model input would be conceivable, which should be investigated in future studies. NNs could be trained with complete and also incomplete datasets and the following predictions could be performed for incomplete datasets. Potentially, NNs could replace the information of missing datasets from alternative datasets.

Additionally, it should be investigated whether it is possible to train different material models with one network architecture. This could potentially result in material card selection by the NN depending on imported experimental test results, which would further reduce necessary expert knowledge. In this way, additional hurdles to the use of FEA in product development would be eliminated since the user would now no longer have to select among hundreds of material cards one appropriate one.

Not least, the prediction based on experimental data for complex material models should be further investigated since virtual datasets are often used for this purpose due to the necessary experimental effort. Thus, possible problems like model errors are often not included in the investigations.

4 CONCLUSION

The continuous development of methods of artificial intelligence and machine learning as well as their application to everyday engineering problems offers new possibilities and potentials to improve and simplify conventional processes in product development. In this article, it has been shown how the direct inverse ML-based material parameter identification method can be applied to the product development process. It has been explained how this method can transform the PDP to achieve increased product quality and cost reduction through the subsequent integration of digital methods. It was explained that the integration of the direct inverse approach into everyday product development already offers advantages such as time and cost reductions, more precise determination of product specifications, and more knowledge-based material selection due to the accelerated execution of accurate finite element analyses. Additionally, potentials were shown that might arise in the future with the integration of the direct inverse method into the PDP and the combination of further digital methods such as shape optimization. These include, for example, individual part-specific component dimensioning in additive manufacturing for widely varying material properties, e.g. polymer recyclates. Consequently, reduced material waste could contribute to a resource-saving PDP. Finally, future research topics were identified.

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