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Automated Hybrid Machine Learning System for Production

Hendrik Mende[a]*, Henrik Heymann[a], Laura Battistella Fiorini[a], Gustavo Schewinski[a], Dennis Grunert[a], Albina Karimova[a], Hamidreza Paria[a], Christian Strobl[a], Robert H. Schmitt[a,b], Thomas Bergs[a,c] *

[a]*Fraunhofer Institute for Production Technology IPT, Steinbachstr. 17, Aachen 52074, Germany*
[b]*Laboratory for Machine Tools and Production Engineering WZL of RWTH Aachen University, Campus-Boulevard 30, Aachen 52074, Germany*
[c]*Manufacturing Technology Institute MTI, RWTH Aachen University, Campus-Boulevard 30, Aachen 52074, Germany*

* Corresponding author. Tel.: +49-241-8904-386. *E-mail address:* hendrik.mende@ipt.fraunhofer.de

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Abstract

Hybrid Machine Learning (ML) models have potential for high performance, as they learn based on data and incorporate existing knowledge. In this work, an automated system is developed which creates the best possible hybrid ML model without Data Science expertise. First, the system architecture is defined including the breakdown of functionalities into a workflow along the sub-components of the system. Then, the system is validated on a use case from optics production, i.e., quality prediction during nonisothermal glass forming. A performance comparison between a baseline ML model with the automatically generated hybrid ML model is demonstrated.

Keywords: Hybrid Machine Learning; AutoML; Optics Production

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1. Introduction

Machine Learning (ML) as a modelling tool in manufacturing has seen a constant growth in the last decade, owing to the versatility and effectiveness of data-driven algorithms and numerous improvements in the field [1]. Neural networks, for example, empowered by modern computing capabilities, excel at solving complex problems. ML-algorithms find extensive utility across various production domains, from predicting product quality to simulating tool design and detecting anomalies within processes. [2]

Nevertheless, despite their performance, many methods such as neural networks are not transparent and informally termed as black-box models [3]. This lack of transparency presents a significant hurdle to process experts unfamiliar with data science, particularly in the development of processes within the production domain. Understanding the relationships between influential factors and response variables through the model, is of great importance to enhance process understanding and advancing knowledge concerning physical relationships and correlations.[4] Here, hybrid models are a solution that holds the potential to support these processes by combining the advantages of ML and expert knowledge in the form of so called white-box (WB) models to solve complex learning tasks [5]. While automated model generation tools, known as AutoML, already exist for purely black-box (BB) models, the absence of a solution for hybrid models is recognized by the authors.

This paper presents a conceptual framework for an automated hybrid ML system designed for the production domain, validated through a nonisothermal glass molding (NGM) use case. NGM is vital in technical optics and thin

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glasses production due to its cost and energy efficiency [6, 7]. Research efforts have aimed at enhancing NGM process quality and understanding through simulations [8], ML-models [9], and optimization methods [10, 11]. NGM involves hot forming of optics or glass products, characterized by nonlinear relationships between parameters, notably temperature and force, impacting product quality. Core glass temperature measurement remains challenging but crucial for deeper process understanding [12]. Modeling final product quality aids in identifying production issues and relationships among process parameters. Expert-based simulations may overlook factors, while ML algorithms demand expertise and large data volumes, posing challenges for SMEs [13]. As a demonstration, nonisothermal glass molding (NGM) is a representative use case for applying hybrid modeling.

The subsequent sections of this paper are structured as follows: Section 2 delves into the state of the art concerning hybrid modeling, encompassing their applications and configurable setups. Section 3 details the proposed system architecture of the *Automated Hybrid Machine Learning System for Production*. This is followed by section 4, which describes the experimental setup of the NGM use case and analyzes the system's application. Finally, section 5 concludes our findings and gives an outlook on the development of the proposed system.

2. State of the art

Hybrid ML models represent a combination of parametric and nonparametric structures, combining the strengths of both methodologies. Parametric models adhere to predefined structures based on prior knowledge, such as mechanistic or phenomenological models (e.g., a rheological model, a simulation, or expert knowledge). On the contrary, the structure of nonparametric models - such as neural networks - is inferred from data. [14] Hybridization offers enhanced model significance by providing both physical insights and a deeper understanding of underlying processes, achieved through the integration of parametric components, which increases interpretability and reduces reliance on extensive datasets. Moreover, hybrid models excel in extrapolation, enabling reliable predictions beyond available data, vital for insights in unexplored process regions. [14, 15]

2.1. Structures of Hybrid Models

Hybrid models can be customized through various combinations and connections of parametric and nonparametric sub-models, offering flexibility in structure and arrangement. These structures are typically either parallel or serial, as depicted in Figure 1. [15] Serial structures are beneficial when certain aspects of the mechanistic model are unknown, with the nonparametric model filling in this missing information. For instance, a hybrid model with a BB-model preceding a WB-model is effective when detailed mechanistic insights are lacking. Here, the BB-model predicts this information based on process inputs and transmits it to the WB-model for computation of the final result. Parallel structures are utilized to rectify mispredictions from one model type, and mixed structures, incorporating both serial and parallel configurations, are feasible approaches to achieve well-performing models, as demonstrated by [16]. [14, 15]

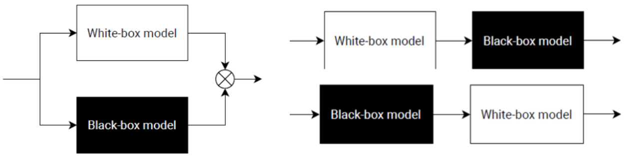

Fig. 1. Three principle hybrid model structures adapted from [14].

Regarding the structure, there is no universally preferred arrangement. The selection of the optimal structure depends heavily on the available knowledge and the quality of information obtained by each sub-model [14]. This choice presents a significant challenge, as there is no single architecture that consistently outperforms others. The decision regarding the preferred arrangement must be carefully evaluated based on the specific requirements and constraints of each use case.

2.2. Hybrid Model Applications

The study by [17] illustrates one of the earliest applications of hybrid modeling, focusing on the dynamic characteristics of fed-batch bioreactors, traditionally challenging to model accurately. By integrating first-principles knowledge with neural networks, the hybrid model showed enhanced robustness and interpretability compared to standard neural network models, while requiring fewer training resources. The hybrid model, detailed in Figure 2, combines a BB- and a WB-model sequentially, with the BB-component predicting cell growth rate using initial process variables as inputs, which is then utilized by the WB-model along with the initial variables to forecast process variable values for the next sampling instant. Empirical tests across various scenarios consistently demonstrated the hybrid model's superior performance in mean squared error (MSE) over the standard neural network approach.

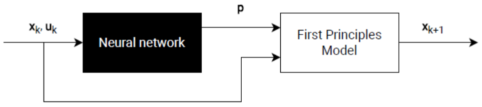

Fig. 2. Serial structure of hybrid model used to determine the kinetics [17]

In their work, the authors of [18] advanced hybrid modeling, achieving comparable performance to standard neural networks in forecasting kappa numbers in pulp mills with significantly reduced training time, indicating the potential for further refinement and application in various industrial contexts. Their hybrid model, depicted in Figure 3, adopts a serial structure, utilizing a WB-model to predict kappa numbers based on kinetics equations and process factors, which are then integrated with additional factors and inputted into a neural network for final kappa number prediction, crucial for assessing pulp quality. Evaluation demonstrated slightly superior performance of the hybrid model over standard neural networks, with half the training time required.

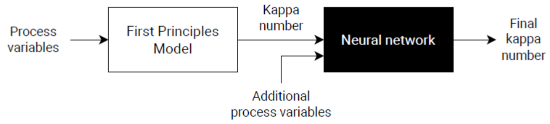

Fig. 3. Serial structure of hybrid model used to predict the kappa number [18]

Reference [16] introduces a hybrid model tailored for predicting undesired friction forces in micropullwinding processes, facilitating proactive prevention measures. Illustrated in Figure 4, this hybrid model combines parametric and nonparametric models in parallel, with another nonparametric model to determine friction force. One nonparametric model predicts winding angle while a causality-driven model provides a parallel output for the angle. Subsequently, the most accurate prediction, along with additional measured data, is fed into a final nonparametric model to predict friction force. This hybrid model surpasses deterministic models and ordinary neural networks, achieving an R-squared value of 0.9576 with a Gradient Boosting Regressor, demonstrating its potential in practical production environments. Despite acknowledging challenges in determining optimal structure, the authors outline three key steps: defining model structure, training BB-model, and analyzing results obtained. [16]

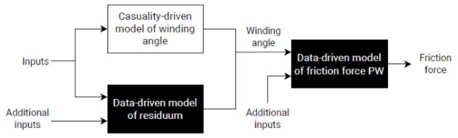

Fig. 4. Structure of hybrid model to predict friction forces [16]

The application of Physics-informed Neural Networks (PINN), which were first presented by [19] in 2019, is frequently examined in the literature on hybrid models. By adding physical restrictions to the loss function, this technique combines parametric knowledge with nonparametric neural networks to improve their interpretability and capacity for generalization. Although PINN models have demonstrated good extrapolation ability and promising results, their implementation is difficult and case specific. It requires developing a mathematical expression representing a physical constraint as a Partial Differential Equation (PDE) to be added to the neural network's loss function. PINN represents a significant concept in hybrid modeling, with demonstrated potential for accurate predictions. [20–22]

Various structures of hybrid models with application in the production context; these structures were created based on the particulars of each use case. Thus, it is necessary to ensure that each particular structural design is considered in an AutoML hybrid system.

3. Proposed System Structure

The Auto*mated Hybrid Machine Learning System for Production*, as illustrated in Figure 5, follows a structured workflow initiating with production data analysis and pre-defined WB-models' requirements. This analysis leads to the generation of potential hybrid model structures capable of fulfilling the modeling task. The configuration process involves two key components: model architecture definition driven by user-provided use case requirements, and model coordination and performance evaluation. In the latter, data is fitted to all hybrid models and their performance benchmarked against defined tasks, with sub-models trained or set up using historical production data. Iterative training occurs through interactions with an AutoML module and the White Box-library, with potential integration with external simulations. Following comprehensive evaluation, the most optimal hybrid model and structure are selected.

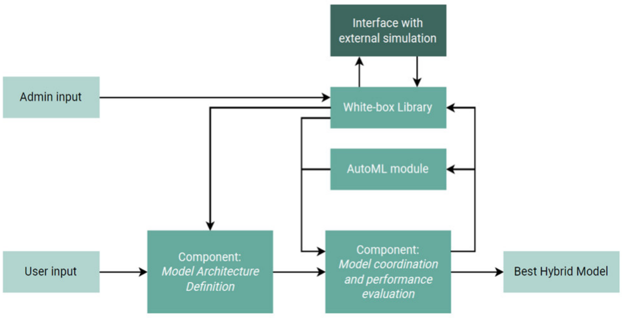

Fig. 5. Workflow for configuring a hybrid model

3.1. White-Box and Black-Box components

The first step in configuring hybrid models is to add models to the WB-Library, which is a repository of all the WB-models that are accessible for a certain process. Process experts take on this responsibility to ensure thorough coverage as they are knowledgeable with the physical behavior and dynamics of the production process. The name, type (external simulation, mathematical model, expert knowledge), the model itself (e.g., equations for mathematical models), necessary parameters or variables (inputs), and output parameters are required information to fully characterize each model entry.

The second part consists of a standard AutoML module that creates ML-models on by itself using historical data. For this, software libraries like autokeras, H2O, and auto-sklearn have been implemented. Both components are integrated as software modules within the software concept.

The software's application unfolds in two phases. The configuration phase entails gathering result requirements and describing the use case via an input mask, configuring, and training the hybrid model with historical data, and making it ready for use. Subsequently, the usage phase involves inputting new process data into the designed hybrid model to obtain predictions of desired values.

3.2. Model Architecture Definition

A pivotal component of the system is the model architecture definition, which explores various structures and configurations without yet considering use case limitations and requirements. Certain restrictions have been made based on the use cases shown from production, to accomplish a reduction in complexity in the current version:

- Only one WB-model is utilized.
- Multiple black box models can be employed.
- Serial configurations shouldn't have two consecutive BB-models.

- Parallel combinations are restricted to one WB-model and one BB-model; two models of the same type cannot be combined.

Considering these premises, the system generates possible hybrid structures, yielding different combinations of serial, parallel, and mixed arrangements.

As per Chapter 2.1, the hybrid model's structure depends on available knowledge, leading to two questions:

- (Q1) Is process data for every parameter needed to construct the WB-model available?
- (Q2) Does the output of the WB-model match the output that the user requires for the whole hybrid model?

Process experts address these questions by refining the configuration workflow and retaining viable layouts. Subsequently, they outline the objectives, inputs, and outputs of the sub-models. Regarding Q1, a BB-model is unnecessary if all parameters required for the WB-model are available as input data, thus the hybrid structure should begin with a single parallel component or WB-model. Conversely, a BB-model may precede the WB-model to predict missing parameters. Regarding Q2, no structural adjustments are needed if the WB-model's output aligns with the user's desired output. However, if they differ, a BB-model following the WB-model or parallel combination predicts the result. Options lacking a BB-model following a single WB-model or parallel component are eliminated. The evaluation process is shown in Figure 6.

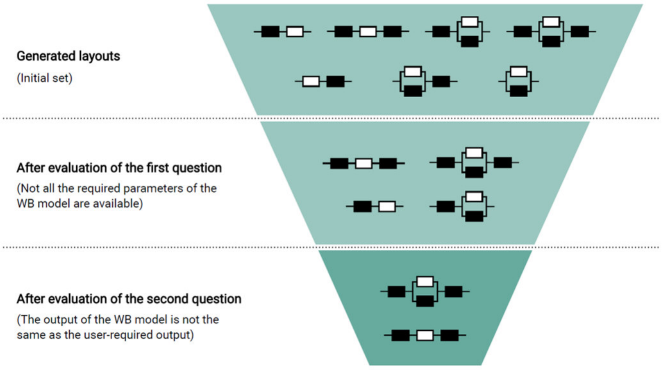

Fig. 6. Evaluation process of generated hybrid model structures after checking parameter availability (Q1) and WB-model output (Q2)

3.3. Model Coordination & Performance Evaluation

The model coordination and training process of the hybrid model are detailed in Figure 7, outlining essential steps for effective training. Unlike the model definition step, which focuses on data description, this phase involves feeding historical data to the sub-models. WB-models are executed solely to gather data for BB-model training, with input data sufficient for WB-models and both input and output data required for BB-models. After this step for all viable hybrid models, performances are compared using common evaluation metrics. Overall, the structured workflow of the system begins with data analysis and user input, leading to the generation, configuration, and evaluation of potential hybrid model structures, ultimately providing a hybrid ML model.

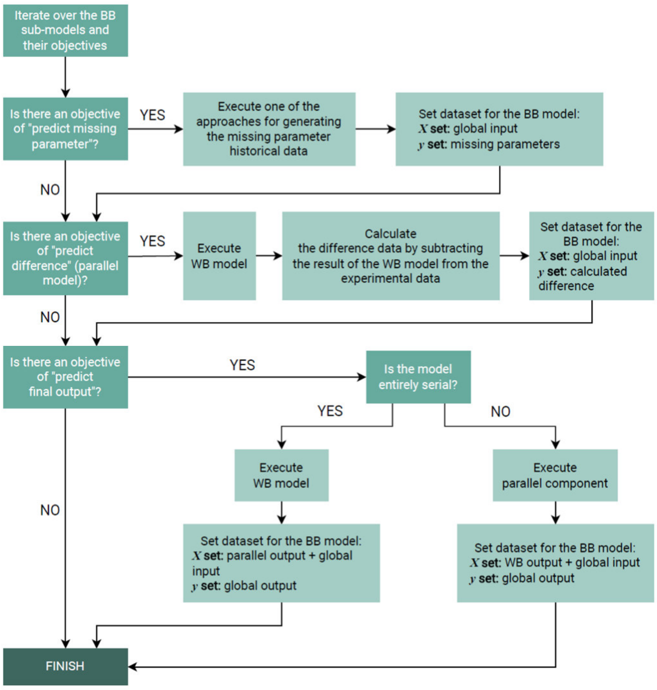

Fig. 7. Proposed training process of a hybrid model

4. Application to Use Case from Optics Production

In the following the application of the proposed *Automated Hybrid Machine Learning System for Production* to a real-world use case in optics production is explored.

4.1. Description of Process and Experimental Setup

For the design of experiments, Latin Hypercube Sampling (LHS) was applied to generate parameter values for the following experiments [23]. The design space included multiple parameters of the lens production process, e.g., heating time, press time, pressing force, upper and lower forming tool temperature. Certain parameter constraints, such as maximum and minimum temperatures, were determined from preliminary experiments. As a result, 500 parameter combinations were defined by implementing LHS.

A nonisothermal horizontal glass forming process (NGM) was employed for lens production. This involved separating the heating and annealing steps from the actual forming process. Firstly, the glass preform was heated separately in an external oven and then transported to the forming tools using a robot arm. Secondly, the preheated glass preform was formed into the desired plano-convex shape. Finally, the molded glass was transferred to an annealing oven, where an annealing step was performed to release the remaining stresses. [24]

To evaluate the process quality, tactile measurements were conducted on the produced lenses using a MarSurf LD 260 Y (Mahr GmbH) profilometer. For each lens, 2D and 3D measurements of the lens surface were taken. The forming tools were measured before and after the experiments to consider possible mold degradation during the experiments. The actual tool measurement data was compared with lens measurement data by filtering profiles, aligning point clouds, and eliminating tilting, centering, and rotation errors. Form deviation and peak-to-valley (PV) values were obtained for each lens.

4.2. Model Configurations for NGM

Definitions of the available WB-models and possible architectures of hybrid models were established. Three different kinds of WB-sub-models were considered: (i) simulation models; (ii) rheological models (such the Maxwell or Burgers models); and (iii) expert knowledge in the form of feature selection based on physical laws. As shown in Figure 8, three feasible structures for the hybrid model were found.

In the first setup, a WB-model (type iii) sits before a BB-model in a serial configuration. Here, the WB-model predicts shape deviation based on a subset of characteristics by using expert knowledge that was taken from the WB-library for feature extraction.

In the second structure, a serial configuration is maintained, but with a BB-model followed by another WB-model. The BB-model predicts unknown parameters for the WB-model (type i), which employs a material model to simulate shape deviation.

The third option combines serial and parallel configurations. Initially, a WB-model conducts feature extraction of prediction data. This information is then provided as input, alongside another WB-model (type i), in parallel. One WB-model simulates shape deviation, while the other predicts the residuum. The outputs are combined to determine the final shape deviation value.

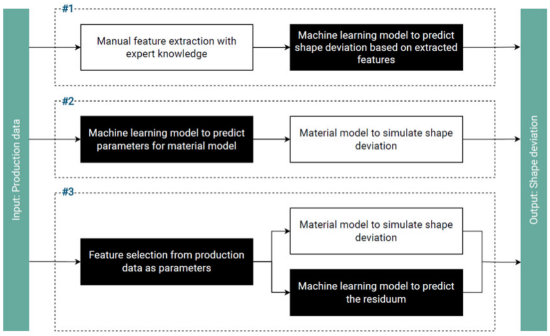

Fig. 8. Estimate of possible hybrid model structures for the use case

4.3. Material Model to Simulate Shape Deviation

Throughout the whole steps in glass molding process, the governing physical phenomena are thermal and mechanical effects which are happening concurrently. Therefore, to simulate the glass molding process accurately, the FEM model needs to consider both concepts simultaneously. To address heat interactions of each molding tool, the thermal model defines the temperature change in each individual part. This model describes convection, radiation, and conduction of each tool together with contact conductance in contact surface of the components. On the other hand, the mechanical model considers the elastic behavior of molding tools, viscoelastic behavior of the glass component, and any mechanical interaction of the tools. The viscoelastic model consists of stress relaxation and structural relaxation during molding in high temperature and later in cooling steps of annealing process. The required coefficients for FEM simulation such as friction, heat transfer, and material coefficients are adopted from previous research works. [25–28]

4.4. Integration of Expert Knowledge

A feature selection routine was developed to streamline the process of selecting crucial features for the hybrid models. This routine utilized time series data collected from individual sensors during tests. To enhance the efficacy of feature selection, expert knowledge was integrated into the preselection of the most significant sensors. Key sensors, including force and temperature sensors, were identified, and incorporated into the WB-library.

Five of the most important features that were manually extracted as part of the baseline model, guided by expert process knowledge are:

- Minimum temperature in proximity to the forming tools
- Area under the curve (AUC) of the temperature in the preheating furnace
- Standard deviation of the temperature near the forming tools
- Maximum pressing force
- Duration of the applied force

These features were identified based on the insights and expertise of domain experts, aiming to capture essential aspects of the production process for effective model training and prediction.

4.5. Results

The hybrid models aimed to predict the PV value of produced optics through regression. Among them, the combination of expert knowledge feature extraction with Lasso regression emerged as the best-performing, with an RMSE of 1.7 µm on the test dataset. This performance is attributed to factors such as abundant experimental data and integration of process expertise from the WB-library. Additionally, similar error metrics between training and test datasets (0.4 µm) indicate effective avoidance of overfitting.

To provide a comparative benchmark, a baseline AutoML model was constructed on the dataset as a pure BB-model. This involved utilizing three available libraries: Auto-Sklearn, Autokeras, and H2O AutoML. AutoML models yielded scores ranging from 5.03 µm to 100.13 µm; nevertheless, there was a significant difference between the test- and training-set, suggesting that the models were overfit. The support vector machine (SVR) model applied by auto_sklearn produced the most reliable and effective model, which showed an RMSE of 11.78 µm on the training dataset and 14.15 µm on the test dataset.

5. Conclusion and Future Work

In conclusion, this paper presents a novel framework for an automated hybrid ML system tailored for the production domain, with validation through a use case from nonisothermal glass molding (NGM). The integration of ML algorithms with expert knowledge, termed hybrid models, addresses the limitations of purely black box (BB) models while leveraging the advantages of both approaches. The proposed system architecture encompasses two key components: *Model Architecture Definition* and *Model Coordination & Performance Evaluation*. The former explores various hybrid model structures considering process requirements, while the latter involves training sub-models and evaluating their performance using historical data. Through a systematic evaluation process, feasible hybrid model structures are identified, addressing constraints such as parameter availability and output compatibility.

Application to the NGM use case demonstrates the efficacy of the proposed approach. Three feasible hybrid model structures were identified, incorporating expert knowledge feature extraction and simulation models. The best-performing hybrid model, combining expert knowledge feature extraction with Lasso regression, achieves excellent performance in predicting peak-to-valley (PV) values of optics produced, with an RMSE of 1.7 μm on the test dataset. This performance is attributed to the integration of process expertise. Comparative analysis with baseline AutoML models highlights the superiority of the proposed hybrid model approach.

Overall, the proposed framework offers a promising solution for addressing complex learning tasks in the production domain, particularly for industries lacking ML expertise. Future research could focus on further refining hybrid model structures and exploring applications in other production processes, leveraging the benefits of both ML and expert knowledge.

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