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Hybrid physics-based and data-driven models for smart manufacturing: Modelling, simulation, and explainability

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ABSTRACT

To overcome the limitations associated with purely physics-based and data-driven modeling methods, hybrid, physics-based data-driven models have been developed, with improved model transparency, interpretability, and analytic capabilities at reduced computational cost. This paper reviews the state-of-the-art of hybrid physics-based data-driven models towards realizing a higher degree of autonomous and error-free operation in smart manufacturing. Recognizing the complementary strengths of pure physics-based and data-driven models, hybrid physics-based data-driven models are categorized as consisting of three types: (1) physics-informed machine learning, (2) machine learning-assisted simulation, and (3) explainable artificial intelligence. The principles and characteristics of these three types of hybrid physics-based data-driven models are summarized to address three aspects of smart manufacturing: product design, operation and maintenance, and intelligent decision making. Finally, the prospective directions and challenges of hybrid physics-based data-driven models are discussed from the perspective of data, scientific insights, interpretability of hyperparameters, and trading off between accuracy and explainability.

1. Introduction

Recently, the rapid advancement of information and communication technologies has greatly accelerated the transformation of manufacturing towards smart, digital, and autonomous manufacturing. Digitalization of manufacturing promotes the collection of data from manufacturing processes and the usage of advanced data analytical techniques to extract information from the collected data. Advanced data analytical techniques based on physical laws or purely data-driven methods have shown the ability to analyze the relationship among the various variables, better revealing the physical mechanisms underlying the manufacturing processes and addressing news challenges in smart manufacturing, which can be illustrated from the perspective of complexity and uncertainty.

Uncertainty denotes the uncertainty of mechanisms/experience, and it is directly correlated with the understanding of mechanisms of the researched problems and the degree of mastering experience. Complexity is the computational complexity that represents the time complexity of computer algorithms, correlating with the complexity of mechanisms in industry and the implementation efficiency of algorithms [1]. Problems encountered in data analytics for smart manufacturing can be classified into four types [1]: low-uncertainty and high-complexity, low-uncertainty and low-complexity, high-uncertainty and low-complexity, and high-uncertainty and high-complexity, as shown in Fig. 1.

Physics-based models and data-driven models perform differently for these four types of problems. On the one hand, physics-based models used to be the primary tool in manufacturing to estimate physical variables and analyze their relationships and address low-uncertainty problems. Commonly used physics-based models include empirical equations, finite element models (FEM), and multi-physics coupling models. Empirical equations describe the relationship between variables using mathematical formulas inferred from experiments, which contributes to observing and analyzing the variations of physics phenomena [2]. Empirical equations which contain limited information about physics are challenged when addressing problems with high complexity because they perform inadequately and lack robustness under complex working conditions due to complex dynamics.

To deal with low-uncertainty and high-complexity problems, simulation models, such as finite element simulations, are constructed to analyze dynamical phenomenon. Finite element simulations approximate solutions to differential equations by decomposing the region to be

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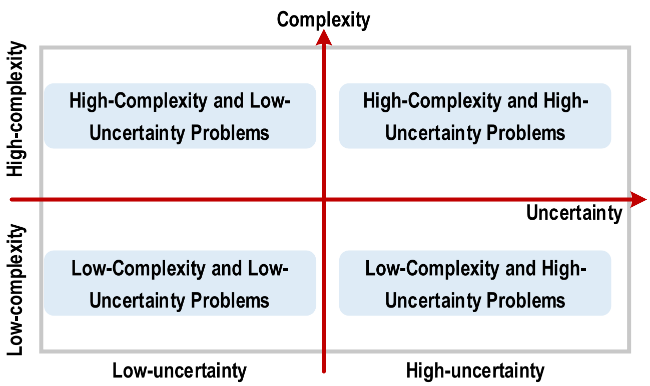

Fig. 1. Classification of researched problems in smart manufacturing.

solved into multiple small elements [3]. Physics-based models illustrate real-world problems using inference with the goal that they can be understood by users, and the solutions are often termed white-box models [4]. Accordingly, these models have been widely accepted. On the other hand, data-driven models, such as machine learning, can address high-uncertainty and low-complexity problems by building the correlation among physical phenomena and predict behaviors of manufacturing systems. Three widely applied data-driven modeling techniques are deep learning, machine learning, and transfer learning [5]. Machine learning techniques extract features from monitoring signals to represent critical information of equipment, and then construct the relationship between handcrafted features and fault types [6,7]. However, conventional machine learning techniques may be challenged when addressing problems with high complexity, such as facial recognition, as their feature extraction ability is limited [6]. In comparison, deep learning can construct end-to-end models with deep structures to explore critical features hidden in signals and address high-uncertainty and high-complexity problems [8].

Several issues need to be considered when applying physics-based and/or data-driven models to data analysis in manufacturing. For physics-based models, high-fidelity finite element simulation means high computational burden. Different from empirical equations and finite element models which focus on information in a single domain, multi-physics coupling models integrate information from multiple domains and consider them simultaneously [9]. High computational burden associated with high-fidelity physics-based models such as finite element simulation, limits the response rate in data analysis. For data-driven models, the black box nature represents a roadblock in their widespread application [10]. Transfer learning extracts fault information from known domains to address issues from other related domains, and can avoid excessive computational time induced by hyper-parameters optimization in complex deep learning models [11]. In general, the inference mechanism of data-driven models is not yet fully understood and interpretable by physics, thus is opaque to users. These issues highlight the importance of constructing data analysis systems by combining physics-based with data-driven models.

In summary, it is important to combine physics with data-driven methods to ensure the transparency, interpretability, and response rate of data analysis systems to realize a higher degree of autonomous and error-free operation in smart manufacturing. Although some papers have illustrated the combining of physics with data-driven methods, most of them only illustrate a certain pattern of the combined methods, such as physics-informed machine learning [12] and explainable machine learning [13]. This paper aims to fill the gap by providing a comprehensive review of the combined methods, termed hybrid physics-based data-driven models (HPDM), and illustrating the improvement of data analysis systems by using HPDM in smart manufacturing. This paper first illustrates the importance of combining physics with data-driven methods from the perspective of complexity and uncertainty of the researched problems in smart manufacturing. By comparing physics-based models and data-driven models, the difference and complementarity of both types of models are analyzed, and the advantages of combining physics with data-driven models are illustrated. The current application scenarios and the prospective opportunities of HPDM in smart manufacturing are also discussed.

The remaining of this paper is constructed as follows. In section, the review methodology of this paper is introduced, and an overview of the current research status of HPDM, the comparison between physics-based models and data-driven models, and the advantages of HPDM are illustrated in Section 2. In Section 3, HPDM for smart manufacturing is summarized and classified depending on the pattern of combining physics with data-driven models. The application scenarios of HPDM in smart manufacturing are presented in Section 4. The future development direction and current challenges of HPDM are discussed in Section 5. Conclusions are drawn in Section 6.

2. Overviews

2.1. Review methodology

The emphasis of this review is placed on journal articles and public reports indexed in global databases, such as ScienceDirect, IEEE Xplore, and Springer link. Recently published papers on HPDM are surveyed according to the keywords, such as ’theory-guided’ [14], ‘physics-informed’ [12], ‘physics-based’ [15], ‘physics-constrained’ [16], ‘simulation-assisted’ [17], ‘physics-guided’ [18], etc. Relevant material is identified and carefully screened. As a result, the materials are divided into three groups: physics-informed machine learning, machine learning-assisted simulation, and explainable artificial intelligence. The flowchart of the review methodology is based on [19].

2.2. Combining physics with data driven models

The combination of physics and data driven has been applied in some fields. In the domain of biomedicine, combining physics with data-driven models effectively improved the ability to explore information from medical images, benefitting the design of more effective treatment protocols [20–23]. In the domain of geosciences and climate, combining physics with data-driven methods contributed to estimating the variation of climate and preventing sudden catastrophe [24–32]. In the domain of additive manufacturing, combining physics with data-driven methods offered outstanding benefits, such as low training time, data-driven decision logic, real-time responsiveness, and uncertainty quantification [28]. Recently, different phrases have been proposed in literature to illustrate the methods combining physics with data-driven models including ‘theory-guided’ [14], ‘physics-informed’ [12], ‘physics-based’ [15], ‘physics-constrained’ [16], ‘simulation-assisted’ [17], and ‘physics-guided’ [18]. Physics improved the physical consistency of data-driven methods [12,14]. Theory-guided data science integrated theory-based models into the modeling, learning algorithm, output samples, and observational data to ensure that data-driven methods were consistent with physics, termed physical consistency [14]. Physics-informed machine learning introduced physical biases into the training samples, model architectures, and inference algorithms of data-driven models to obtain physics consistent solutions [12]. Physics-based machine learning developed low dimensional representations of high-fidelity simulation results as the training samples of machine learning [15]. Physics-constrained machine learning applied partial differential equations to constrain the optimization of data-driven models and improve convergence rates [16]. Moreover, many papers emphasized constructing hybrid models by utilizing physics-based models to guide the construction of data-driven models. Simulation-assisted machine learning embedded simulation models into machine learning models’ training samples, hypothesis set, algorithm, and final hypothesis to guide the construction of data-driven models

[17]. Physics-guided machine learning fused physics-based models into the preprocessing, model design, and regularization of data-driven models to guide the construction of hybrid models and ensure interpretability [34]. In summary, the common methods of combining physics with data driven are to embed physics into the two aspects of data-driven models, data and model construction, as illustrated in Table 1.

2.3. Comparison between physics-based models and data-driven models

As the development of intelligent analysis technologies, both physics-based models and data-driven models can analyze the complex relationships between input and output. However, physics-based models possess strong interpretability by considering physics compared with data-driven models. A comparison between data-driven models and physics-based models is shown in Fig. 2.

Data-driven models utilize the samples of known variables to reversely infer the relationship between the known variables, which scarcely considers physics. The construction of data-driven models includes data preprocessing, model selection, setting parameters, and model optimization. The preprocessing methods, such as normalization and down sampling, are adopted to process the samples of known variables to ensure their quality, not considering problem-specific physics. The type and characteristics of the samples are regarded as important references to model selection. In the period of setting parameters, parameter search methods, such as grid search, are applied to determine the parameters and ensure the accuracy of data-driven models. However, these methods hardly consider the accuracy increasing mechanism of data-driven models during parameter searching. According to the selected data-driven models, optimization algorithms are selected to minimize the error between prediction and actual observations. Overall, the construction of data-driven models highly correlates with the samples of known variables, which scarcely contributes to the understanding of the inner logic of model construction. However, black-box data-driven modeling can obviously improve the speed of modeling, decrease the computational burden, and contribute to constructing lightweight models to describe the relationship between physical variables.

Different from data-driven models, physics-based models infer the relationship between known physical variables according to physics. The construction of physics-based models includes determining the target variable to be solved, selecting the hypothesis set, setting parameters, and solving the model. The first step of building the relationship between variables is to determine the variable to be solved by considering domain knowledge. Next, the hypothesis set which partly reflects the relationship between the known variables and the variable to be solved is selected by considering physics. The parameters of the hypothesis set, such as physics parameters and boundary conditions, are combined with the hypothesis set to solve the target variable. Compared with data-driven modeling, physics-based modeling is capable of improving understanding of the inner logic of model construction, which enables researchers to partly control the model construction [34]. But, the accuracy of simple physics-based models, such as empirical equations, inclines to be influenced by the complex working conditions in manufacturing. High-fidelity simulation including massive information about physics always leads to unaffordable computational burden and decreases the response rate of data analysis systems.

Table 1
Common methods of combining physics with data driven in literature.

Approaches	Reference	Data	Model construction
Theory-guided data science	[14]	✓	✓
Physics-informed machine learning	[12]	✓	✓
Physics-based machine learning	[15]		✓
Physics-constrained machine learning	[16]		✓
Simulation-assisted machine learning	[17]	✓	✓
Physics-guided machine learning	[18]		✓

There exists a complementarity between physics-based models and data-driven models, as shown in Fig. 3. By integrating physics into data-driven models, data-driven models can be transparent and partially interpreted by physics, which helps humans understand them furtherly. Moreover, by integrating data-driven models into physics-based models, their advanced inference ability is exerted to simplify the construction and solution of high-fidelity simulations, which contributes to reducing computational burden and improving computation speed. As a breakthrough in data analytical techniques, HPDM combines physics-based models with data-driven models based on complementarity. HPDM has the merits of both physics-based models and data-driven models and overcomes the drawbacks of purely using data-driven models or physics-based models.

3. Methodology

HPDM can improve the analytic capabilities, interpretability, transparency, and response rate of data analysis systems, which plays an important role in addressing the challenges carried by the sea of industrial big data and realizing a higher degree of autonomous and error-free operation in smart manufacturing, as shown in Fig. 4.

First, the sensors deployed on the users' equipment collect monitoring signals to construct HPDM. According to the complementary nature of physics-based and data-driven models, this paper categorizes HPDMs as three types, including physics-informed machine learning, machine learning-assisted simulations, and explainable artificial intelligence. Physics-informed machine learning aims to embed physical laws into the construction of data-driven models to improve the model interpretability. Machine learning-assisted simulations apply data-driven methods to simplifying simulation models and approximating solutions, which contributes to improving the computational efficiency of physics-based models. Explainable machine learning focuses on exploring the post-hoc explanation for improving the explanability of the training samples, model inputs, and prediction results to increase the transparency of data-driven models.

Second, the obtained HPDM is applied to constructing interpretable, explainable, and rapid-response data analysis systems to carry out the four types of analytics of manufacturing systems: descriptive analytics, diagnostic analytics, predictive analytics, and prescriptive analytics [8]. Descriptive analytics aims to describe the conditions of a manufacturing system in the current or past time. Diagnostic analytics is to judge the current state of a manufacturing system and the causes which induce the current state. Predictive analytics refers to predicting the future conditions of a manufacturing system. Prescriptive analytics proposes solutions to forthcoming conditions. With the outstanding analytics provided by interpretable, explainable, and rapid-response data analysis systems based on HPDM, the knowledge-base for smart manufacturing is advanced.

Thirdly, with the advanced analytics enabled by HPDM, the transformation of manufacturing from the current practice to a highly autonomous and error-free smart process can be enabled. The benefits include reduced operational costs, continued satisfaction of changing consumer demands, improved productivity, reduced machine downtime, enhanced observability, improved product quality, accurate assessment of the health conditions of working equipment, and informed decision making.

3.1. Physics-informed machine learning

Physics-informed machine learning essentially integrates physics into data-driven models to improve interpretability so that experts can partly understand their construction, as shown in Fig. 5. Overall, physics can be embedded into three essential aspects of data-driven models, including data, modeling, and loss functions.

High-quality training samples play an important role in constructing

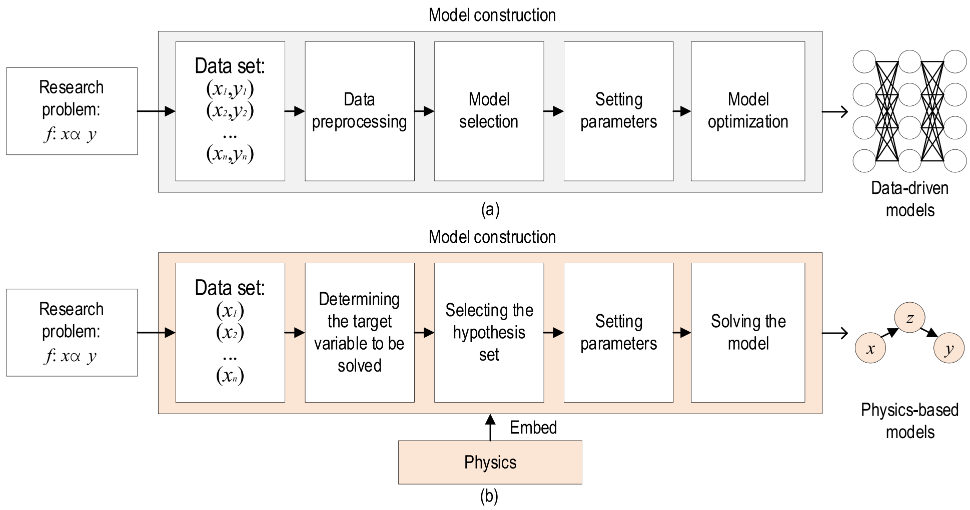

Fig. 2. The comparison between (a) data-driven models, and (b) physics-based models.

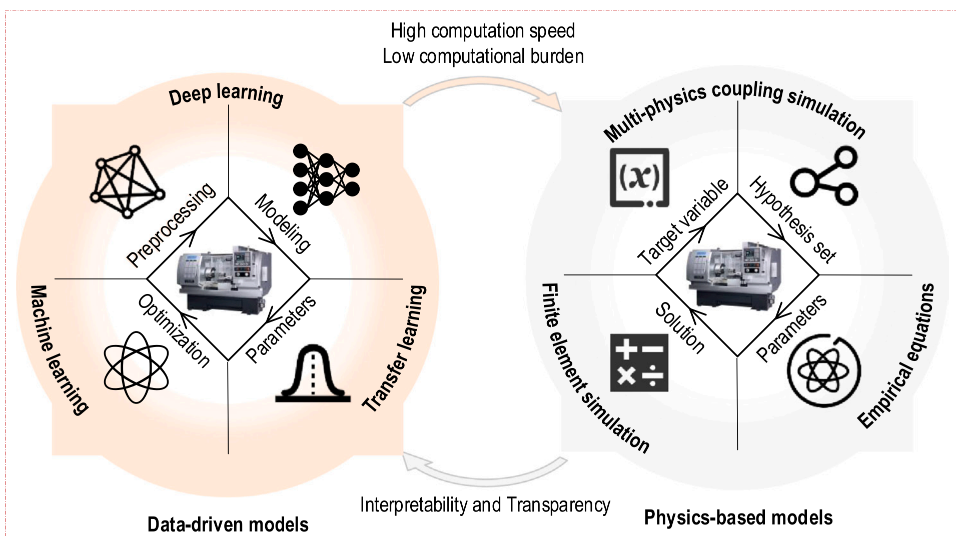

Fig. 3. Complementary relationship between physics-based and data-driven models.

the relationship between physical variables using data-driven models. Data pre-processing techniques, such as normalization, can transform irregular data types into the ones that can be processed by computers conveniently. Feature extraction methods, such as Fast Fourier Transform [35] and wavelet analysis [36], can extract problem-specific features by considering domain knowledge. To furtherly improve the interpretability of data, physics-informed machine learning employs data carrying physical meaning and consistent with physics as the training samples of data-driven models, such as the calculation results of empirical equations and simulation. Different from data-driven methods, empirical equations are constructed based on physics mechanisms. Therefore, the calculation results of empirical equations are interpretable and consistent with physics. Simulation models, a type of physics-based models with complexity and accuracy, integrate massive physics information to ensure the simulation results to be interpretable and consistent with physics. Furtherly, some scholars proposed to utilize physical characteristics to constrain physical variables instead of applying specific models [37,38].

For modeling, physics can be applied to select proper data-driven models and model design. On the one hand, there exist some essentially interpretable data-driven models describing the relationship between variables in a way that humans can understand, such as decision trees [39] and linear regression [40]. Linear regression can estimate a physical variable by assigning weights to the other multiple ones [40]. Based on historical data and experience, decision trees allow experts to assign multi-dimensional quantitative or qualitative labels corresponding to the various aspects of a research object and describe the condition of the research object based on these labels [39]. On the other hand, physics can be applied to design the structure of data-driven models to improve interpretability. Using interpretable inference mechanisms of physics-based models to guide data-driven modeling to construct hybrid models has been a novel pattern of model design. A representative pattern, termed data-driven hybrid equivalent dynamic modeling, perfectly fused the inference ability of data-driven models and the interpretable modeling of physics mechanism to design the structure of data-driven models [41]. Besides, some papers applied physics mechanism to design the internal components of data-driven models. A typical example was the physics-guided convolutional neural network (CNN) which applied physics to design the convolutional kernel [42]. An emerging structure, termed recurrent neural network (RNN) based cumulative damage models, applied a group of empirical equations to improve the internal unit and was deployed to calculate the changes of physical variables [43].

Traditional loss functions of data-driven models emphasize

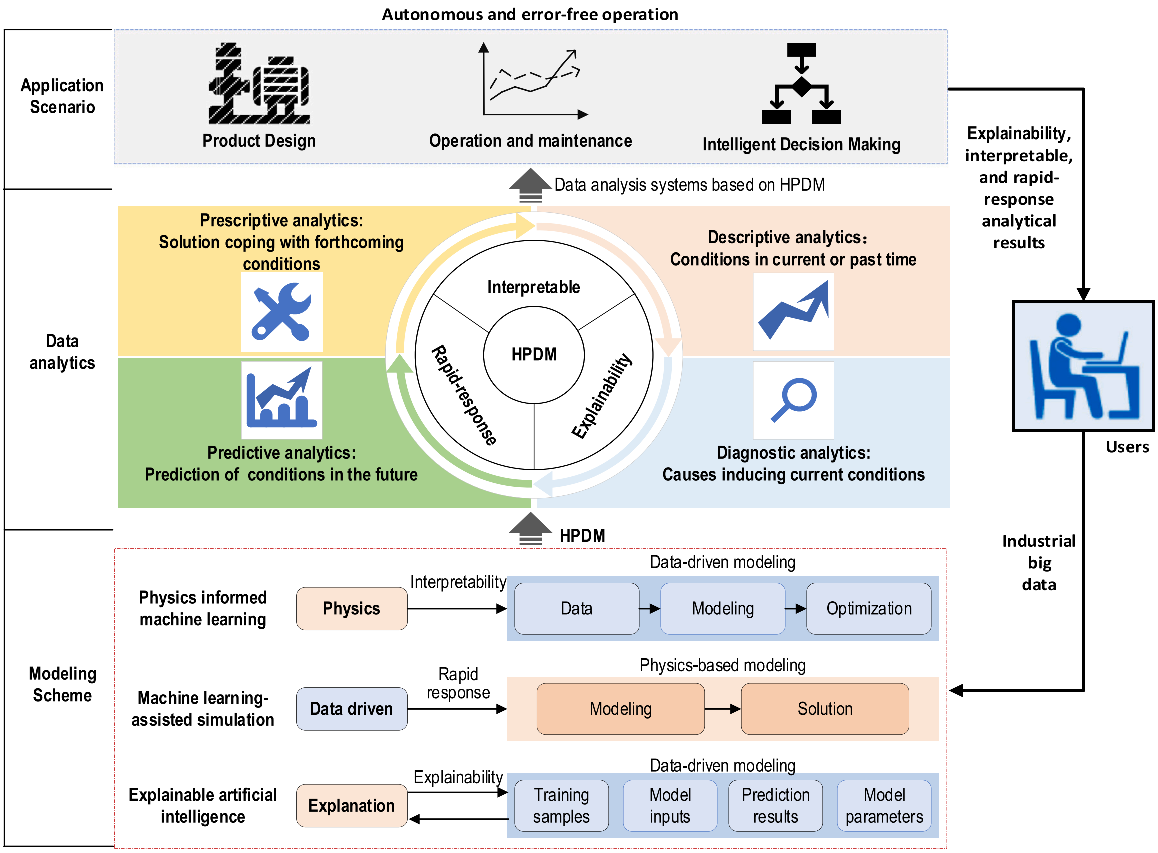

Fig. 4. The scheme of using HPDM to construct explainable, interpretable, and rapid-response data analysis systems with advanced analytic capabilities to realize a higher degree of autonomous and error-free operation in smart manufacturing.

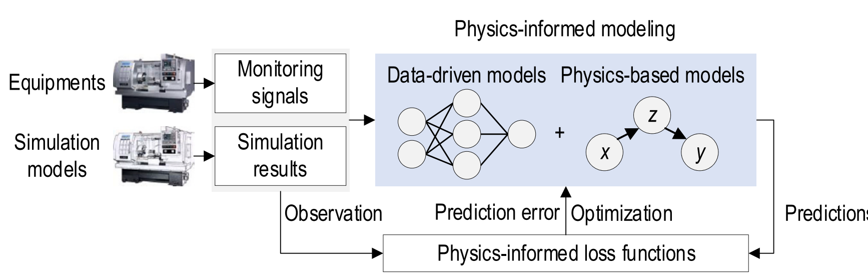

Fig. 5. The scheme of physics-informed machine learning.

decreasing the loss between estimation and actual observations and ignore the inherent physics of the researched problems, resulting that the obtained model and results may not be consistent with physics. In response to this challenge, physics is applied to construct physics-informed loss functions to constrain the data-driven models into the space with physics consistency. Physics applied to modify loss functions can be categorized into two types, including the relationship between physical variables and the characteristics of physical variables. The prediction results of physical variables to be solved were constrained by embedding the relationship between known physical variables and physical variables to be solved into loss functions [44–46]. A typical example was physics-informed neural networks which employed boundary and initial conditions to constrain the solutions of partial differential equations, and the sum of the prediction loss was applied to construct the loss function [47]. Embedding the characteristics of physical variables into loss functions aimed to reserve the physical inconsistency of predicted physical variables into the loss function of deep learning models, termed physics guided loss function [48], and then the physical consistency of deep learning models and prediction results could be improved by minimizing prediction loss calculated by the physics-guided loss function. The common methods of physics-informed machine learning are summarized in Table 2.

3.2. Machine learning-assisted simulation

Physics-based simulation plays an increasingly important role in manufacturing with a great demand for model fidelity. However, achieving high fidelity requires the simulation models with fine-scale spatiotemporal resolution of the system of interest, and thousands of computing cores of simulation lead to enormous computational burden [49]. The computational burden constrains the application of high-fidelity simulation in many scenarios with rapidly simulation requirement, such as model predictive control. To relieve the computational burden of simulation, data-driven methods are applied to construct reduced-order models and find approximate solutions to simulation models, as shown in Fig. 6.

Model reduction seeks to construct reduced-order models that provide accurate approximations of the full model solutions with reduced

Table 2
The methods of physics-informed machine learning.

Approach	Methods	Reference
Embed physics into network input	Data preprocessing	Normalization, Band-pass filtering, Down sampling, Data cleaning.
	Feature extraction methods	Harmonic wavelet packet transforms [36], FFT [35]
	Simulation results	Reynolds-averaged Navier-Stokes simulations [37], Large-eddy simulation [38]
Embed physics into models	Model selection	Linear regression [40], Decision tree [39]
	Model design	Physics-based convolutional neural network [42]
Embed physics into loss functions	The relationship between physical variables	Physics-informed neural network [44–47]
	The characteristics of physical variables	Physics-guided loss function [48]

computational complexity [50]. Model reduction includes non-intrusive model reduction methods and intrusive model reduction methods [51]. The intrusive model reduction methods require full knowledge of the governing equations and the discretized full models of dynamical systems. However, the solutions and discretization are not available due to the enclosed software for simulation, which constrains the application of the intrusive model reduction methods. To address this problem, the non-intrusive model reduction methods integrate data-driven methods into model reduction to infer approximations to the full model solutions from snapshots samples [50–52]. The non-intrusive model reduction methods based on projection-based methods transforms the snapshot samples of high-fidelity simulation models into low-dimensional representations [15]. The low-dimensional representations are regarded as the training samples for data-driven modeling. Data-driven methods characterized by machine learning simulate dynamic systems as black boxes by building the correlation between input and output, which provides an important platform to learn the mapping between the low-dimensional representations. Specially, the proper orthogonal decomposition (POD) based on singular value decomposition projects the quantities of interest as POD basis and POD coefficient associated by polynomial response surface models to obtain the mapping between the measurement quantities of interest and the capability quantities of interest. Besides, POD can be combined with other data-driven methods, such as Bayesian classifier [53], neural network [15], and least-squares minimization [52,54,55], to decrease the computational burden and increase the response rate of a computing system.

Data-driven models not only can learn the mapping between low dimensional representations but also can be integrated into numerical methods of high-fidelity simulation models [17]. Differential equations are important to illustrate the physical phenomenon that represents the relationship among independent variables, unknown functions, and the derivatives of unknown functions with respect to independent variables. Some numerical methods, such as finite element analysis, are essentially to solve the differential equations. To reduce the computational burden of solving the equations, the neural network was proposed to assimilate temporal and spatial information and approximate solutions to the partial differential equations [56]. The derivatives of the approximate solutions with respect to independent variables are calculated to construct the PDE residual. The PDE residual is applied to construct the objective function of the neural network for optimization.

3.3. Explainable artificial intelligence

Explainable artificial intelligence explores hidden knowledge about data and model construction by explaining the correlation among inputs, outputs, training samples, and data-driven models. Different from physics-informed machine learning and machine learning-assisted simulation where physics is regarded as an information source except for data, explainable artificial intelligence extracts post-hoc explanations after training using data-driven models, as shown in Fig. 7. Then, the post-hoc explanations are analyzed to obtain knowledge or understanding about data and model construction for adjusting model hyperparameters and configuration of training samples to improve the transparency and interpretability of data-driven models. Explainable artificial intelligence can be illustrated from two aspects, data and modeling.

From the perspective of data, explainable artificial intelligence can evaluate the influence of input features on predictions by perturbing or occluding input samples, and thus increase the transparency of data. A representative example is local interpretable model-agnostic explanations which construct an interpretable model to calculate the feature importance of perturbed inputs to classify results [57]. Similar methods, such as prediction difference analysis [58], deconvolutional networks [59], and Shapley additive explanation [60], can analyze the influence of modifying input features on the outputs of deep learning models. Besides, the correlation between training samples and testing samples can be analyzed using perturbing or occluding. Estimating the influence of changing training samples on the prediction error of testing samples can determine the most influential training samples to ensure the accuracy of data-driven models and obtain more insights about the training samples [61].

From the perspective of modeling, explainable artificial intelligence analyzes the semantics of hidden layers of data-driven models by finding input samples which can maximize the activation of the hidden layers, termed activation maximization [62]. To improve the interpretability and transparency of neural networks, activation maximization is applied to a deep convolutional network to find representative input samples [63]. The representative input samples can be regarded as prototype samples for model construction. The similarity between the prototype samples and the feature maps of convolutional neural networks is regarded as the weights of the outputs to improve the interpretability

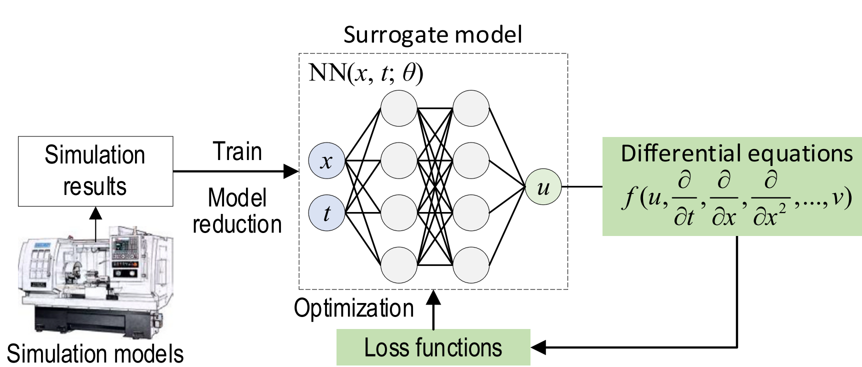

Fig. 6. The scheme of machine learning-assisted simulation.

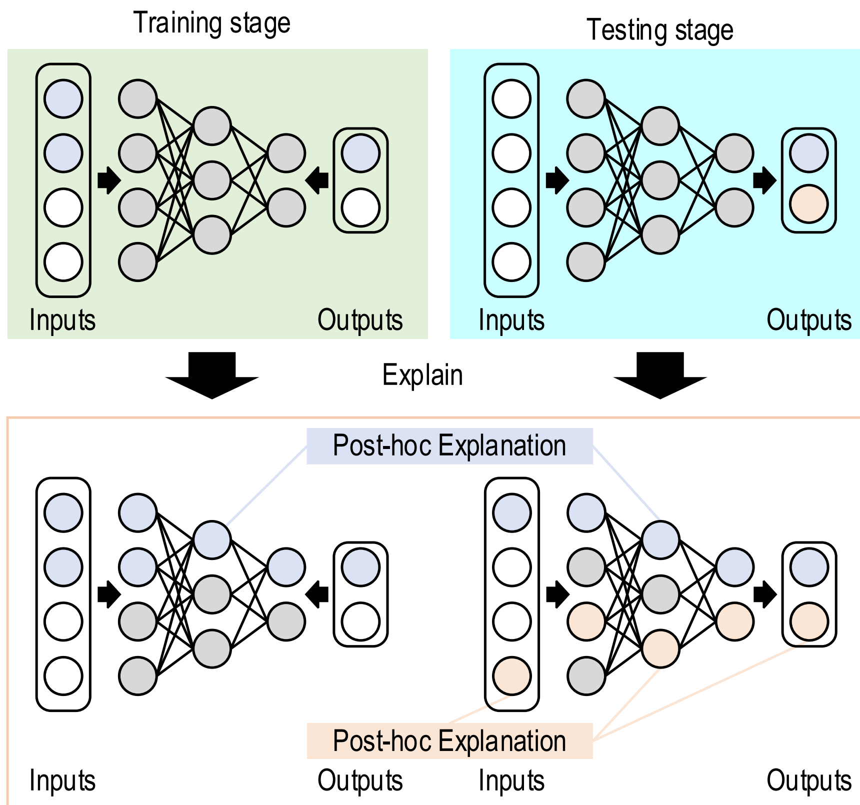

Fig. 7. Illustration of an explainable network structure.

and transparency of inference [64].

4. Representative applications

The requirement of transparent, interpretable, and rapid-response data analysis systems with advanced analytic capabilities accelerates the realization of a higher degree of autonomous and error-free operation in smart manufacturing. Various application scenarios of HPDM and corresponding literature are summarized, as presented in Table 3. The main application of HPDM in the life cycle of products in manufacturing industries is divided into three categories: product design, operation and maintenance, and intelligent decision making, and is discussed in this section.

4.1. Descriptive analytics for product design

Product design in smart manufacturing mainly depends on the construction of an accurate simulation model to describe the designed products accurately [122,123]. Relying on the accurate description provided by simulation models, designers can clearly understand the deficiencies of the products or equipment, and continuously modify the design schemes to improve product quality and accuracy [124]. Moreover, simulation models are deployed to test the performance of the products and improve the overall design scheme to reduce operation and maintenance costs. Finite element method (FEM) is a classical simulation technique that divides the entire region into massive sub-regions and calculates the approximate solutions to the differential equations in each sub-region [56]. However, FEM-based simulations are operated along with high computational expense due to the massive solutions of the differential equations, which is unacceptable for small-scale enterprises. Moreover, simulation models hardly apply dynamic data to keep being updated and evaluating the condition of working equipment, leading to a deviation of the operation of equipment from the objective of product design.

To avoid the excessive computational burden of high-fidelity simulation, an emerging direction in product design is to construct interpretable physics informed machine learning models to approximate the relationship between physical variables. Physics-informed machine learning is applied to solve discrete-time and continuous-time models such as the Allen-Cahn equation and the Schrodinger equation, which obviously reduces the cost for solving the simulation models [56]. To constrain the cost for constructing the simulation models and meanwhile ensure the prediction accuracy, the simulation results of tubular reactor models of reactive flows were projected into a low-dimensional space, and the operators of the nonlinear systems were inferred by the least-squares optimization [51]. Physics-informed machine learning can estimate the difference between the simulation models. The simulation results of Reynolds-Averaged Navier-Stokes and Direct Numerical Simulation were applied to compute the discrepancy between training flows and test flows on flow physics, which effectively avoided unnecessary simulation modeling [65].

Table 3
The mainstream application scenarios and corresponding literature of HPDM.

Methods	Application scenarios	Reference
Physics-informed machine learning	Product design	[37,65–72]
	Operation and maintenance	[42,43,48,73–85]
	Intelligent decision making	[86–93]
Machine learning-assisted simulation	Product design	[15,49–52,54,66,67,71,94–102]
	Intelligent decision making	[103–111]
Explainable artificial intelligence	Operation and maintenance	[60,112–121]

4.2. Diagnostic and predictive analytics for operation and maintenance

In conventional manufacturing, operation and maintenance immensely rely on physics-based modeling to detect and predict equipment faults [125]. But limited physics can hardly cope with complex working conditions and the sea of industrial big data. Furtherly, dynamic physics parameters influence the accuracy of physics-based modeling, which increases the difficulty of operation and maintenance in manufacturing. In the era of smart manufacturing, massive monitoring signals in manufacturing processes promote the application of data-driven technologies in fault diagnosis and prediction [126]. Fault diagnosis finds existing faults in complex equipment by analyzing collected signals from sensors. Fault prediction predicts the deterioration of mechanical components or equipment, and the prediction results are regarded as an important reference for determining a maintenance plan. However, traditional data-driven models suffer from poor interpretability and are difficult to be deployed in practice.

Physics-informed machine learning can improve the interpretability of data-driven models for operation and maintenance. As an application of embedding physics into training samples, an interpretable domain adaptation for fault diagnosis of locomotive bearings was constructed by combining simulation datasets and actual measurement datasets [126]. This interpretable domain adaptation mined fault information from simulation datasets to improve the interpretability of the input samples and eliminated the influence of training sample size on the performance of fault diagnosis. Compared with fault prediction purely based on physics-based modeling or data-driven modeling, a physics-based fleet deterioration prediction model was embedded into a cumulative damage model and combined with data-driven mapping to achieve the interpretable deterioration prediction of a fleet [78,79]. For wind turbines, similar modeling methods were applied to the estimation of bearing fatigue [80]. Explainable machine learning can improve the transparency of data-driven methods and verify the consistency between data-driven models and physics mechanisms. Local interpretable model-agnostic explanations were applied to explain the neural network for fouling resistance predictions and demonstrated that the predictions were consistent with the calculation results of physics-based models by randomly perturbing the inputs of the neural network [117].

4.3. Prescriptive analytics for intelligent decision making

To avoid decision making influenced by the subjective factors of humans, such as emotion, intelligent decision making was proposed by combining human decision making with artificial intelligence to predict the demands of users, provide critical information, and suggest prescriptive action plans [127]. However, traditional intelligent decision making scarcely considers the physics mechanism in practical, which affects the interpretability of intelligent decision making systems and threatens their penetration in smart manufacturing. An emerging direction for intelligent decision making is to combine physics mechanisms with data-driven models to improve the credibility and interpretability of intelligent decision-making systems.

Physics-informed machine learning provided a new pattern of intelligent decision making for digital twin workshops, with improved interpretability and response rate by integrating simulation with data-driven analysis [86]. Digital workshops were built to receive real-time information from physical workshops and construct the simulation models of physical workshops to achieve interconnection and interoperability between digital workshops and physical workshops. Then, the production data of physical workshops and the simulation data of digital workshops were analyzed by data-driven models to determine production plans. However, conventional simulation models are time-consuming, which disturbs the interconnection and interoperability between digital workshops and physical workshops. To achieve fast response and low computation time in intelligent decision-making systems driven by digital twin, data-driven model-reduction was proposed to construct an offline and online intelligent decision-making system [105]. In the offline stage, polynomial response surface models were regarded as the surrogate model of high-fidelity simulation models to construct the relationship between measured quantities of interest and capability quantities of interest. In the online stage, the surrogate model was applied to estimate the capability of real-time measurements and support real-time decision making.

5. Discussion

As the complexity of manufacturing processes and equipment increases, constructing interpretable, rapid-response, and transparent data analysis systems with advanced analytic capabilities to realize a higher degree of autonomous and error-free operation in smart manufacturing has become a great challenge in current manufacturing. HPDM provides a potential platform to endow current manufacturing stronger analyzing ability in coping with more complex situations. However, there exist some issues in the current application of HPDM under the condition of current manufacturing. The existing problems and prospective development trends of HPDM are discussed from four aspects, including data, scientific insights, interpretability of hyperparameters, and trading off between accuracy and explainability.

5.1. Data

The 5 V attributes (Velocity, Volume, Value, Variety, and Veracity) of big data indicate that new analysis tools will be needed for effective data processing [128]. While methods such as feature extraction, synthetic minority oversampling [129] and image synthesis [130] can be applied to exploring the “Value” aspect of big data, the other 4 V attributes that represent the nature of big data still present significant challenges to HPDM [131]. Sufficient training data is important to ensure the robustness of data-driven models and explore the latent relationship among the physical variables. The “Volume” and “Velocity”of big data result from the increasing deployment of sensors on machine equipment with edge-computing capabilities to construct an information transmission pipeline for real-time signal acquisition and situation awareness, which however induces additional operation cost [56,132]. The “Variety”of big data reflects on the reality of multi-modality data acquisition and the need for multi-level and multi-resolution data fusion, which represents a challenge to the computational infrastructure and cost of HPDM. Often times, sensor placement at optimal locations may be constrained by space and other environmental conditions [33,133]. Although simulation can facilitate data-driven modeling, the computational cost of high-fidelity simulation represents a physical limitation. Virtual or soft sensing is a technique that enables state inferencing at a location by processing physical sensing data obtained at another location, thereby addressing the “Veracity” characteristic of big data [133].

5.2. Scientific insights

An essential premise to construct an accurate HPDM model is to gain valuable scientific insights into the researched manufacturing system. The construction of HPDM requires not only well-versed practitioners in data-driven models but also a thorough understanding of the scientific insights. Insufficient or inaccurate scientific insights hardly ensure the interpretability of obtained HPDM models, which indirectly affects the accuracy of describing the relationship between physical variables. Existing methods of exploring scientific insights, such as numerical simulation and empirical equations, bring various challenges to HPDM. For example, in the domain of predictive maintenance, a numerical simulation of the continuous deterioration of parts in a manufacturing system directly leads to incredible computational cost and increases the difficulty of searching for faults depending on simulations. Complex working conditions severely influence the robustness of the parameters in empirical equations. Inaccurate physical parameters hardly reflect the relationship between the monitored physical variables and deterioration. In summary, it is urgent to develop a convenient and low-cost method to explore accurate and sufficient scientific insights from a manufacturing system.

5.3. Interpretability of hyperparameters

According to the theory of physics-informed machine learning, embedding physics into data-driven models can improve interpretability. But some hyperparameters in the modeling and optimization of data-driven models cannot be interpreted by physics. For example, the number and size of layers in a neural network during the setting of model hyperparameters in data-driven modeling [13], and the learning rate and batch size during the setting of hyperparameters in the optimize algorithms. The hyperparameters with poor interpretability may lead the data-driven model to suffer from a local minimum. Both methods can help to address this issue. Firstly, selecting interpretable algorithms, such as decision trees, can avoid the hyperparameters with uncertainty but it is difficult to cope with overly complex problems [39]. Secondly, explainable artificial intelligence can be adopted to analyze the correlation between hyperparameters and data [62–64]. In summary, improving the explainability or interpretability of data-driven models is a priority because it makes the models more robust, and consistent with physical laws and principles, thereby facilitating a broad acceptance of data-driven models in real-world applications by the manufacturing and engineering communities.

5.4. Trading off among accuracy, explainability, and computational power

The tradeoff between model accuracy and explainability is a multifaceted problem and can be affected by multiple factors, such as sensing methods and computational power, etc. It implies that more explainable HPDM may be less accurate [134]. While high model accuracy may be achieved by black-box models such as random forests or artificial neural networks, their lack of explainability makes it difficult to understand their working mechanism and the rationale of their predictions. In comparison, white-box models such as decision tree and linear regression are readily understandable but lack predictive capacity. While integrating physics into data-driven models can improve the explainability of data-driven models, HPDM may not be thoroughly explainable due to the nature of data-driven models. Trading off between accuracy and computational power also implies that users may tend to accept a slightly less accurate result with substantially reduced computational burden in practical applications. A new approach termed approximate computing has been proposed to modify the semantics of relevant algorithms and assign them with the desirable accuracy and necessary computational power [135,136]. Currently a gap exists in the literature that reveals the explicit relationship between explainability and computational power. Therefore, it is necessary to develop methods for selecting proper HPDM to address different requirements on accuracy, explainability, and computational power in data modeling and analysis.

6. Conclusions

HPDM provides a novel approach to address the challenges facing conventional modeling when dealing with industrial big data. HPDM unlocks the remarkable amount of physics information into advanced data analysis to improve the interpretability, transparency, response speed, and analytic capabilities of data analysis platforms and to realize a higher degree of autonomous and error-free operation in smart manufacturing. A framework is proposed to categorize HPDM as three types, including physics-informed machine learning, machine learning-assisted simulation, and explainable artificial intelligence. Physics-informed machine learning aims to embed physics into the model construction of data-driven models to improve their interpretability. Machine learning-assisted simulation exerts the rapid modeling of data-driven models to surrogate the simulation models and approximates the solutions, which improves response rate and decreases computational burden. Explainable artificial intelligence explains the correlation among inputs, outputs, training samples, and data-driven models to increase the transparency of data-driven modeling. By surveying the studies applying HPDM in manufacturing, it is concluded that HPDM contributes to improving product design, operation and maintenance, and intelligent decision making.

Future work in HPDM for smart manufacturing is envisioned to be a synergistic integration of HPDM with the design of cyber-physical systems. Specifically, constructing explainable, interpretable, and rapid-response data analytics is key to transforming manufacturing systems into smart, digital, and autonomous systems. The technique of Digital Twins plays an essential role in providing a digital thread for smart manufacturing, and has received extensive attention in recent years [137,138]. One of the envisioned future research directions is to enable Digital Twin by HPDM to promote machine-to-machine interconnection and interoperability with explainable, interpretable, and rapid-response data analytics, to ultimately realize deep fusion of physics and industrial big data.

Declaration of Competing Interest

The authors declare that they have no known competing financial interest or personal relationships that could have appeared to influence the work reported in this paper.

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