



Mechanistic artificial intelligence (mechanistic-AI) for modeling, design, and control of advanced manufacturing processes: Current state and perspectives

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ABSTRACT

Today's manufacturing processes are pushed to their limits to generate products with ever-increasing quality at low costs. A prominent hurdle on this path arises from the multiscale, multiphysics, dynamic, and stochastic nature of many manufacturing systems, which motivated many innovations at the intersection of artificial intelligence (AI), data analytics, and manufacturing sciences. This study reviews recent advances in Mechanistic-AI, defined as a methodology that combines the raw mathematical power of AI methods with mechanism-driven principles and engineering insights. Mechanistic-AI solutions are systematically analyzed for three aspects of manufacturing processes, i.e., modeling, design, and control, with a focus on approaches that can improve data requirements, generalizability, explainability, and capability to handle challenging and heterogeneous manufacturing data. Additionally, we introduce a corpus of cutting-edge Mechanistic-AI methods that have shown to be very promising in other scientific fields but yet to be applied in manufacturing. Finally, gaps in the knowledge and under-explored research directions are identified, such as lack of incorporating manufacturing constraints into AI methods, lack of uncertainty analysis, and limited reproducibility and established benchmarks. This paper shows the immense potential of the Mechanistic-AI to address new problems in manufacturing systems and is expected to drive further advancements in manufacturing and related fields.

1. Introduction

Manufacturing is an imperative part of the global economy accounting for 10-30 percent of the gross domestic product in major industrialized countries (West and Lansang, 2018). Historical examples also show innovations in manufacturing nurture key advances in the automotive, aerospace, electronics, and biomedical industries such as 3D bioprinting of tissues and organs (Murphy and Atala, 2014). Particularly, recent advances have moved manufacturing toward design freedom and flexibility allowing the production of highly optimized and individualized parts while remaining cost-effective even for low-volume productions. However, many manufacturing processes are known for their intricacies in changing material shapes and properties.

As a prevalent challenge in manufacturing, we face complex interactions between materials, setups, and energy sources, while the underlying physics is not fully understood. High-dimensional spatio-

temporal behaviors are common in manufacturing applications, and critical responses happen in length scales that are orders of magnitudes apart. As an example, in metal-based additive manufacturing, the interactions between the laser beam and material particles happen in micro-scale, the melt pool dynamics, grain, and porosity evolution occur in meso-scale, and mechanical and thermal behavior appear in macro-scale. While significant progress has been made to accurately simulate these multiscale behaviors using numerical simulations, conventional methods are often prohibitively time- and resource-consuming, especially for cases where an iterative solution is needed (e.g., inverse problems, robust design, uncertainty analysis). To exacerbate the problem, manufacturing systems are prone to noise, disturbance, and unknown hidden variables which make the process difficult to accurately predict. The behavior of manufacturing systems is known to vary even between similar machines or for one machine over time. As a result, the task of decision-making and understanding manufacturing

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processes has remained a daunting engineering effort.

At the same time, manufacturing practices have undergone a digitalization paradigm. This trend can be evidently seen in the strategic road maps across the globe such as the Industry 4.0 framework introduced by Germany, the “Manufacturing USA” institutes in the US, and the “China Manufacturing 2025” strategic plan in China, all of which emphasize systematic digital data collection and large-scale networking and communication capabilities to advance manufacturing systems. Putting these pieces together, one can see that manufacturing systems generate data with continuously increasing quality and variety, and these data sources are valuable assets and should be utilized to advance current capabilities.

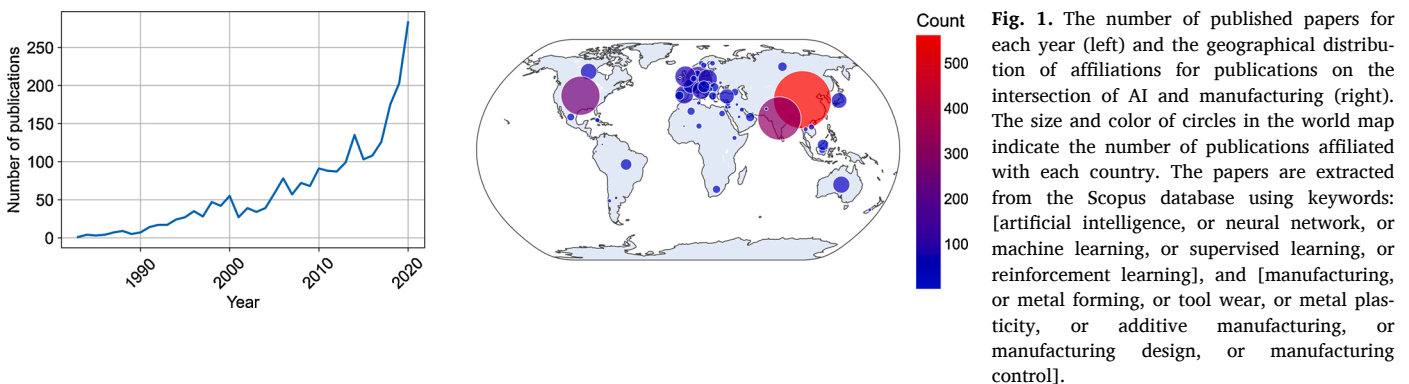
In recent years, Artificial Intelligence (AI) has shown significant progress in automating activities that are associated with human thinking, such as planning, decision making, and problem-solving. An over sixfold increase in the number of publications from 2015 to 2020 (Zhang et al., 2021) and an estimated 15.7 trillion-dollar worth of economy in 2030 (PwC, 2021) are only a few indications of the vast existing and future impact of AI in both academia and industry. AI solutions are capable of processing large-scale data from a wide range of sources, including images, text, audio, 3D geometries, to name a few. As a result, we observe a surge in AI-enabled approaches to enhance prediction, design, and control capabilities of advanced manufacturing processes that leverage the recent trend of manufacturing digitalization and large-scale data acquisition platforms. The increasing popularity of investigating AI methods in manufacturing applications as well as the geographical distribution of publications can be observed in Fig. 1. This cross-disciplinary research area attempts to address critical manufacturing challenges such as improving quality variability and process efficiency and enabling high-dimensional design for tailored material and geometric properties, with the potential to drastically alter the capabilities of these multi-billion-dollar industries. AI methods provide an exciting alternative to many conventional computational methods in manufacturing as they offer high predictive flexibility with fast inference time. Additionally, AI tools are often compact and easier to maintain compared to their conventional counterparts which can involve large code bases with tens of thousands of lines of code.

Despite the many benefits of AI-enabled tools, three key shortcomings hinder the widespread adoption of such tools in manufacturing: (1) unavailability of large enough high-quality data, (2) limited generalization to unseen samples, and (3) lack of interpretability. Developing useful databases from raw information is expensive for complex engineering tasks as such databases need to be carefully processed and curated to minimize the impact of mislabeled instances, imbalances, outliers, and noises. Furthermore, the behavior of manufacturing machines can change over time as machines age, which results in a continuous and costly process of data preparation. AI methods often overfit the data provided to them during the training process, meaning that they exploit the database imbalances and noises to resemble the training samples too closely. The overfitting reduces the accuracy of the solution for new data, especially when new data has a different

distribution compared to the training database. Therefore, a naive implementation of AI methods can easily violate the physical principles of the modeled phenomenon. Developing generalizable solutions is a core effort of AI researchers and practitioners; however, the state-of-the-art methods often fall short of the outside-of-training accuracy required in precise engineering problems. Lastly, AI solutions are often treated as black-boxes and offer limited tools to trace the reasoning behind their decision-making patterns. While interpretability might not be a critical factor in applications such as advertising recommendation systems, unreliable action in manufacturing plants can have devastating financial and safety consequences. Therefore, explainability is another important feature of solutions in manufacturing.

To address the above-mentioned challenges, we advocate Mechanistic-AI methods, in which mechanism-driven principles of manufacturing processes and engineering insights are embedded into AI solutions to increase their data efficiency, generalizability, and explainability. A schematic of the Mechanistic-AI framework is illustrated in Fig. 2. This framework covers multiscale and multiphysics modeling, which is complemented by AI methods to simplify model calibration, validation, and mesh generation. Moreover, the known physical mechanisms could inform AI methods for accurate predictions (i.e., physics-informed learning), and the AI methods, in turn, can be used to discover new mechanisms from experimental data (i.e., data-driven discovery). As a data-centric framework, high-quality high-resolution experimental data with appropriate mechanistic feature engineering and data processing is required for model validation and AI training. The physics-informed AI and well-validated physics-based models, in turn, generate more data. Therefore, Mechanistic-AI provides an interconnected framework between the three components of physical mechanisms, AI methods, and data, which enables a new generation of modeling, design, and control in manufacturing. In this article, we review notable advances in Mechanistic-AI methods in manufacturing systems, introduce a corpus of promising approaches that have not been applied to manufacturing yet, and lay out our vision for influential future directions in this field. We note that the multiphysics modeling with model calibration and validation is beyond the scope of this study. For those topics, interested readers can refer to the reviews by Guna-segaram and Steinbach (2021) and Wei et al. (2021).

In recent years, several publications have reviewed various aspects of AI in manufacturing. Li et al. (2017) discussed a system-level architecture for integration of AI in smart manufacturing facilities and the role of key parties, governments, and technologies in the formation and future of the intelligent manufacturing industry. Sharp et al. (2018) deployed natural language processing (NLP) to extract trends and insights from a corpus of 4000 literature related to machine learning (ML) in manufacturing applications and identified decision support, lifecycle management, and digital knowledge management as important applications of ML in manufacturing literature. Wang et al. (2018) presented a technical summary of deep learning algorithms (such as CNN, RBM, Autoencoder, and RNNs) and their applications in manufacturing quality inspection, fault assessment diagnostics, and defect prognosis.



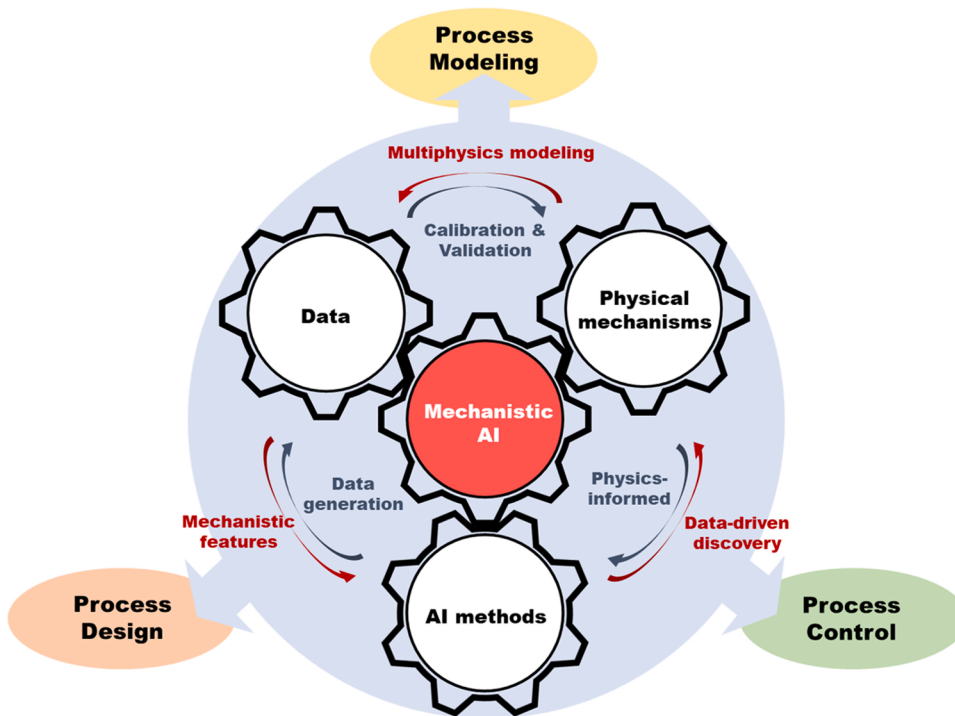


Fig. 2. A schematic of Mechanistic-AI for advanced manufacturing processes, including the building blocks and their interactions. Two cycles connect the Mechanistic-AI building blocks. The red arrows represent a cycle of the information flow: physical mechanisms can create data via modeling techniques, data can be used to train AI methods with appropriate mechanistic feature processing, and AI methods can discover new physical mechanisms by combining experimental data (i.e., data-driven discovery). The dark blue arrows represent a reverse cycle: physical mechanisms can inform AI methods (i.e., physics-informed machine learning), AI methods can create more data, and data can be used to calibrate and validate mechanistic models to elucidate physical mechanisms. The Mechanistic-AI enables scientific-driven process modeling, design, and control. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Gao et al. (2020) identified four building blocks of the life cycle of manufacturing data as data collection, data processing, data learning, and data security and elaborated various methods to tackle current challenges within each item. Arinez et al. (2020) adopted a system-process-material hierarchical plant organization and reviewed the literature to incorporate AI decision-making and analytics tools within and across manufacturing hierarchical levels. A review dedicated to AI tools health monitoring in manufacturing systems can be found in Zhao et al. (2019). Zhang and Gao (2021) summarized recent advances in data processing and curation techniques in manufacturing systems such as denoising, outlier detection, imputation, balancing, and annotation.

Our review article distinguishes itself by providing a new perspective on approaches that transform generic AI techniques into Mechanistic-AI solutions that offer better interpretability and reliability, enable mechanisms discovery, and handle various types of heterogeneous manufacturing data. In what follows, we introduce various classes of manufacturing data and data sources in Section 2. Section 3 provides a discussion on combining physical knowledge and data-driven methods for modeling and discovery in manufacturing processes. We discuss mechanistic feature processing (Section 3.1), physics-informed modeling methods in manufacturing (Section 3.2), and data-driven discovery in manufacturing (Section 3.3). Later, we investigate and categorize several AI methods in manufacturing that are targeted toward design and control tasks in Sections 4 and 5, respectively. Finally, we conclude this article with a summary of promising future research directions for Mechanistic-AI in manufacturing in Section 6.

2. Manufacturing data

2.1. Manufacturing data types and databases

A key trend over the past decade is widespread digitalization across many fields fueled by the availability of inexpensive sensing devices. In manufacturing, digitalization trends, e.g., cyber-physical systems and Internet of Things (IoT) (Lee et al., 2015), have increased the visibility and accessibility to information and drastically changed the amount, quality, diversity, and richness of available manufacturing data.

Manufacturing generates a wide spectrum of heterogeneous data which can be broadly categorized into three different types of (1) experimental data, (2) simulation data, and (3) engineer/user data.

The development of novel sensors to measure complex behavior of materials and manufacturing systems with high accuracy and frequency is an ongoing research area. Additionally, many sensing technologies have matured, leading to lowering equipment costs and ease of availability. As the result, various measurement technologies and sensing methods have become more standardized components of modern manufacturing pipelines from controlling and monitoring during the manufacturing process to test and analysis methods after the products are manufactured. These experimental sources provide data on the material and manufacturing processes across several time and length scales. Some of the popular sensing methods and their data types are compiled in Fig. 3. As it can be seen, manufacturing produces a wide range of in-situ and ex-situ data including scalar measurements in static or time-series forms (such as load cells, vibration, acoustic, fracture, and fatigue data), geometry data (such as point clouds in optical scanning), video data (such as measurements from DIC, IR, and X-ray), and static image data (such as data from X-ray diffraction, scanning electron microscopy, and electron backscatter diffraction). Increasingly, several of such sensing data are compiled together to reduce uncertainty in measurement or to collect a more complete set of the attributes of manufacturing systems. For example, Muhammad et al. (2021) combined X-ray computed tomography (CT) and DIC methods to record detailed microstructural features and local strain evolution and characterize deformation responses of additively manufactured samples.

Advances in numerical simulation methods such as finite element method (FEM), computational fluid dynamics (CFD), and lattice Boltzmann method (LBM), along with the increasing computational capacity generated another source of valuable data stemming from fundamental physical laws. Designs and manufacturing process plans are digitalized through CAD and CAM models, providing detailed information about the geometry, desired tolerances and surface qualities, design intent, and process execution. Additionally, engineers and users, while a source of a smaller portion of data, are a unique source of information in manufacturing plants and provide invaluable manual demonstrations, know-hows, and reporting discrepancies and irregularities (Waterman,

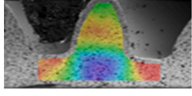
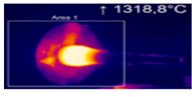
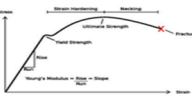
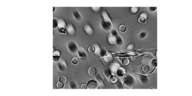
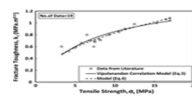
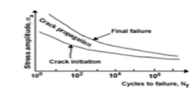
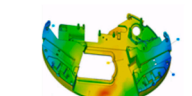
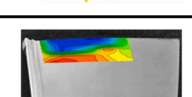
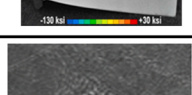
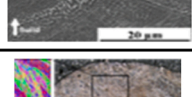
		Sample Data	Observed Feature
In-Situ Measurement Techniques	Digital Image Correlation (DIC)		Strain, displacement
	IR Camera		Temperature
	Load Cells & Extensometer		Force, strain
	X-Ray Imaging		Particles, melt pool, porosity
Ex-Situ Property Measurement Techniques	Fracture Toughness		Absorbed energy
	Fatigue		Fatigue failure
	Optical Scanning		Geometry, point cloud
Ex-Situ Microstructure Characterization	X-Ray Diffraction		Residual stress, composition
	Scanning Electron Microscopy		Structure, grain, phase, porosity
	Electron Backscatter Diffraction		Grain, phase, texture

Fig. 3. Samples of in-situ and ex-situ measurement and material characterization techniques common in manufacturing. This data includes scalar, time-series, point cloud, and image/video measurements.

2017). At the same time, some research is dedicated to the development of efficient knowledge management systems in manufacturing to create, link, maintain, and update heterogeneous manufacturing data, such as studies done by Ko et al. (2021) and Lu et al. (2018). For example, Lu et al. (2018) proposed a four-tier framework consisting of data, information, knowledge, and application. In their framework, a bottom-up analysis is used to extract engineering knowledge and a top-down method is proposed for goal-oriented active data generation.

High-quality databases and benchmarks are imperative for the adoption of AI in manufacturing. Such benchmarks allow scientists to meaningfully track the progress of the field and compare different methodologies, which is nearly impossible if each study is performed on a separate database. Additionally, publicly available databases lower the barrier to research and deploy AI systems as they can significantly reduce the time-consuming and expensive data gathering and curation steps of the AI development life-cycle. Fortunately, in recent years, we

observe the emergence of various databases with applications in manufacturing.

Several public databases provide a wide range of 3D manufacturing-related geometries in various formats such as CAD files, images, and depth maps. ABC geometric database (Koch et al., 2019) contains 1.75 million CAD files for industrial designs. MVTec ITODD (Drost et al., 2017) is developed for industrial object detection tasks and includes 28 objects and 3500 labeled scenes resulted from two 3D sensors and three grayscale cameras. T-LESS (Hodan et al., 2017) provides 50K images for 6D pose estimation with over 30 industry-relevant objects. Online communities such as Thingiverse (Thingiverse. and com,2021., 2021) have accumulated large-scale collections of designs for additive manufacturing parts, which are used to create curated databases by other studies. Thingi10k (Zhou and Jacobson, 2016) contains 10,000 3D printing models in 72 categories and over 4000 tags. Berman and Quek (2020) collected over a million 3D files, images, and metadata for

additive manufacturing parts and published their database as Thingi-Pano. HowDIY website (Berman et al., 2021) is developed not only as a collection of 3D printing designs but also as a platform to provide collaborative support and computationally-guided tools in various steps of 3D printing. A current limitation of such geometric databases for manufacturing applications is that they are mostly designed for generic plastic 3D printing, lack process-specific information (e.g., support structure and toolpath), and do not cover a broad enough range of manufacturing processes. Some recent geometric databases target specific design and manufacturing applications. For example, Biked (Regenwetter et al., 2021) is a database of 4,500 bicycles that includes the individual components, bike class, and numerical design parameters.

Researchers have also invested in developing databases that incorporate the performance of manufacturing processes, notable examples of which are described here. Sundar and Sundararaghavan (2020) developed a database of over 300K simulated microstructures that are resulted from various permutations of tension, compression, and rolling in different directions. This database allows for data-driven investigations to find the relationships between the manufacturing process sequences and the microstructure evolution. Oak Ridge National Laboratory (ORNL) (Scime et al., 2021) released a dataset containing layer-wise powder bed images from three different powder bed printing technologies: laser powder bed fusion, electron beam powder bed fusion, and binder jetting. The dataset was mainly designed for anomaly defects detection using image segmentation or other computer vision techniques. Several databases are published that connect additive manufacturing process conditions and part performances. NIST Additive Manufacturing Metrology Testbed (Lane and Yeung, 2019) provides melt pool monitoring data for ten nickel-based superalloy 625 (IN625) parts with varying scan strategies. NIST AM-BENCH database (Levine et al., 2020) published extensive in-situ and ex-situ measurements (e.g., part deflection, residual strain, melt pool geometry, part tensile properties) for metal and polymer materials. Air Force Research Laboratory (AFRL) AM modeling challenge series data (Cox et al., 2021) provided experimental data at macro- and micro-scale including manufacturing process parameters, residual strain, geometry, microstructural details, and stress-strain behavior. The Additive Manufacturing Materials Database (<https://ammd.nist.gov/>) is a collaborative database that contains information about the material properties, machine parameters, build design, in-process, and post-process data points. These growing attempts to establish rich manufacturing databases can greatly

facilitate Mechanistic-AI methods to find complex manufacturing mechanisms between heterogeneous data types.

2.2. Manufacturing data platforms

Cloud manufacturing can further facilitate and automate the database generation for both proprietary and non-proprietary data sources. Although several different definitions are available in the literature (Siderska and Jadaan, 2018), cloud manufacturing can be defined as a cloud-based platform that collects manufacturing resources from providers online, analyzes collected resources, and offers the various tools and suggestions on manufacturing processes to customers. The term “cloud manufacturing” first appeared in literature in Li et al. (2010) and since then it has gained significant research interests. Notable research on the cloud manufacturing concepts and their implementations are reviewed by Siderska and Jadaan (2018) and Bouzary and Chen (2018).

Fig. 4 illustrates the architecture of cloud manufacturing proposed by Esposito et al. (2016) that consists of 4 layers: manufacturing resource layer, virtual resource layer, service layer, and application layer. The manufacturing resource layer refers to the local facilities that manage production, shipping, operational tasks. The virtual layer contains virtual models and simulation tools of physical resources that ceaselessly produce data to construct a multi-resource database. This data can be used for the optimization of the production cycle and providing recommendations to customers. On top of the virtual layer, the service layer oversees the scheduling and monitoring of the manufacturing process. Finally, the application layer offers a web-based user interface that visualizes tasks performed in the cloud platform.

Despite great advances in the concepts and application protocols of cloud manufacturing, most of them rely on centralized cloud systems and suffer from information transparency and data security. In recent years, decentralization of cloud manufacturing with blockchain technology is trending in the literature, such as Aghamohammadzadeh and Fatahi Valilai (2020) and Barenji (2021). The fundamental idea of this research path is to establish a highly secure blockchain platform for the multi-resource databases that allows providers and customers to match, negotiate transactions, and establish contracts.

Zhu et al. (2020) proposed an Ethereum-based cloud manufacturing platform to solve a benchmark problem that entails 939 job requests from 100 users. They used the k-nearest neighbors (KNN) algorithm for the service composition and successfully mediated 934 jobs. Yu et al.

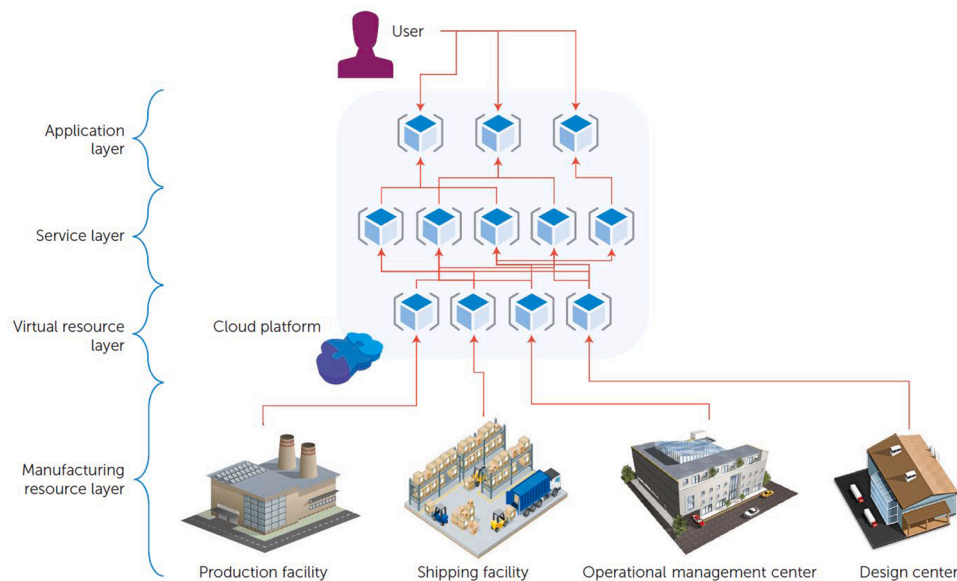


Fig. 4. Layered architecture of cloud manufacturing which includes manufacturing resource, virtual resource, service, and application abstractions (Esposito et al., 2016).

(2020) developed a blockchain-based cloud manufacturing architecture combined with a particle swarm optimization (PSO) solver for the service composition problem. Wang et al. (2021) reported an architecture of blockchain cloud manufacturing that utilizes machine learning techniques such as support vector machine (SVM) and neural network for service composition tasks. Zhang et al. (2021) studied a blockchain consensus protocol to reduce the energy consumption during the Proof of Work (PoW) process, leading to a higher transaction speed and sustainable cloud manufacturing platform. Many blockchain ecosystems are originally designed to transfer a small amount of transaction data, which is not compatible with cloud manufacturing transactions that involve a large volume of manufacturing data. To address this issue, Hasan et al. (2021) developed a middleware software architecture inside the Ethereum network that can store and transfer larger manufacturing data. Such technologies in cloud manufacturing enable the creation of highly secure, anti-tampering, traceable, and transparent multi-resource and multi-fidelity databases for further usage in AI methods.

3. Mechanistic-AI in manufacturing modeling and discovery

For decades, trial-and-error experiments and physics-based modeling were deployed to model various aspects of manufacturing processes, including material properties and product quality. However, trial-and-error approaches are often time-consuming and expensive due to the vast number of process and material parameters, as well as the high expense of experimental tests. Physics-based modeling methods provide many tools to understand complex mechanics in manufacturing processes. But, leaning on physics-based modeling alone can be insufficient in many challenging manufacturing problems for several reasons:

- The accuracy of the popular simulation tools (e.g., FEM) largely depends on the mesh quality. Therefore, manufacturing applications can require extremely fine mesh structures to properly simulate intricate material behaviors, which consequently leads to high computational demand (Francois et al., 2017).
- Formulating the governing equations and solver settings is a non-trivial task due to the multiscale and multiphysics nature of manufacturing processes and their complex boundary conditions.
- Experimental data are generally used for calibration and validation, which requires significant manual engineering, instead of seamlessly embedding them into simulation tools. This disconnection motivates finding the next generation of integrated simulation approaches to better understand complex mechanisms in manufacturing.

Data-driven approaches come into play as promising alternatives considering the increase in data accessibility and parallel computing power. But, data-driven approaches rely on a vast amount of labeled high-fidelity data, which can be difficult to obtain through experiments or simulations. This hinders the wide application of data-driven methods in manufacturing modeling. To exploit the power of data-driven approaches, classical physics-based modeling, and experimental data, we advocate for utilizing Mechanistic-AI for modeling and discovering physical mechanisms in manufacturing.

There are two fundamental components in an AI solution: a machine learning model and the data to train the model with. Both of these components can be reformed to convey the mechanistic aspects of a manufacturing process; hence, creating a Mechanistic-AI approach. Physical insights can be embedded into training data by employing a host of techniques such as mechanistic feature selection and exploiting data invariants, as detailed in Section 3.1. At the same time, the machine learning model can be augmented with physical knowledge of manufacturing processes by how the solution is structured, the formulation of the model, as well as the training process. These advancements are elaborated upon in Section 3.2. We also discuss a third aspect of AI-enabled modeling approaches, known as system identification, which allows the discovery of fundamental physical laws from data, as

explained in Section 3.3.

3.1. Mechanistic feature processing

Successful application of any AI framework largely depends on the nature and relevance of the features considered. Meaningful features are particular helpful in establishing process-structure-property relationships (DebRoy et al., 2018) and designing and optimization of manufacturing processes (Yoshimura, 2007) as these tasks require high explainability and generalizability. Processing raw training data into features that are most efficient in representing relevant aspects of a manufacturing task can drastically improve the suitability of the AI solution for resolving realistic manufacturing problems. Therefore, mechanistic feature processing can play an important role, irrespective of the data types, i.e., experimental, simulation, or user data. Generally, the purpose of feature processing in machine learning is to select the most important features out of many in order to make the training process easier or faster. Here, we refer to mechanistic feature processing as data selection and manipulation techniques that utilize mechanistic or physical insight of manufacturing processes to do the same. Particularly, we introduce two classes of solutions to achieve this goal: (1) selecting most important and physically meaningful features in a given task, and (2) using the existing invariants in the data to transform or augment the data. These two solutions are elaborated in the following subsections.

3.1.1. Mechanistic feature selection and importance analysis

An inappropriate feature selection generates information with a high noise-to-signal ratio and low correlation to target, which impedes the training process and reduces the accuracy and generalizability of AI solutions. The underlying physical aspects of a manufacturing process can inspire meaningful and mechanistic feature selection in various tasks. Current literature in manufacturing lacks a unifying framework for the selection of mechanistic features; rather, the selection process is highly domain-specific with heavy reliance on the experience of experts in the field. Here, we highlight several inspiring examples of mechanistic features across the manufacturing fields.

In additive manufacturing processes, various interacting mechanisms affect the performance of parts. Gu et al. (2021) proposes the concept of Material-Structure-Performance Integrated Additive Manufacturing (MSPI-AM), which integrates parallel multi-material, multi-functional, and multiscale materials design and production. The authors discuss many relevant mechanistic features for realizing an advanced hybrid manufacturing system. For example, to produce a multi-functional and multi-material part, the feature selection requires identifying an appropriate lattice structure, crystal orientation, composition, and material gradient distribution.

Geometric features can play an integral part in analyzing manufacturing performance. Mycroft et al. (2020) used geometric features extracted from CAD such as voxel map, thickness, mesh complexity, and curvature to predict the Hausdorff printability measure for the powder bed fusion process. Note that while in some manufacturing processes, such as forming, global aspects of the geometry significantly affect the distribution of forces, in other processes, such as machining, the geometric effects are mostly local. Therefore, understanding the direct and indirect region of influence of each physical energy source can assist in selecting important features in manufacturing tasks. In geometry optimization tasks, i.e., topology optimization, mechanistic features such as toughness, force-displacement curves, mass, and geometric parameters can be used to efficiently optimize complex geometries (Gongora et al., 2020).

Metallic alloy material design tasks can benefit from thermodynamic and structural properties as the mechanistic features because they control the property of the manufactured alloys. Such features become critical to assess physical phenomena that are hard to observe experimentally such as surface energy (Hebert, 2016). Tian et al. (2021)

showed that high-throughput density functional theory (DFT) features are helpful to select a suitable alloy composition for a desired mechanical performance. In microstructure analysis tasks a significant body of research suggests utilizing statistical metrics as material descriptors (Huber et al., 2020). The key idea behind these works is to convert a microstructure image with multiple phases into an n-point correlation function, where the probability of finding a specific phase is represented as a function of relative distance. Other metallurgical data such as Electron Backscatter Diffraction (EBSD) features, average grain size, and volume fraction of other phases are also used as features in multiple studies, such as Baturynska et al. (2018) and Herriott and Spear (2020).

Once a set of features are selected, relative importance analysis can reveal additional physical insights. As the result of importance analysis, one can remove low-impact features, which simplifies and accelerates the training and prediction processes. Tree-based methods, such as Random Forest, naturally provide statistical importance analysis of the input features (Biau and Scornet, 2016). Two measures of importance are commonly used in the Random Forest. The first measure, i.e., accuracy-based importance, is based on the change in accuracy if the feature is excluded. The second measure, i.e., Gini-based importance, is based on the decrease of Gini impurity (or node purity) when a feature is chosen to split a node. Both measures can be used to order mechanistic features and identify dominant features in advanced manufacturing processes. Xie et al. (2021) identified important temperature ranges for ultimate tensile strength (UTS) from infrared temperature data in additive manufacturing. They found two dominant temperature ranges in process-induced thermal histories, and those ranges have a significant influence on the resulting UTS of the printed Inconel 718 material. The dominant ranges were identified purely from experimental data without prior knowledge but they surprisingly coincided with the theoretical results. As shown in Fig. 5, the first temperature range, 1212.99–1365.35 °C, align with the solidus and liquidus temperatures of the Inconel 718, and the second important range, 654.32–857.47 °C, is related to γ' and γ'' precipitate formation temperature during solid-state transformation. Du et al. (2021) evaluated the Gini-based importance of the mechanistic features on balling defect in additive manufacturing. They concluded that the Marangoni number and solidification cooling time are the two most important features that describe the balling effect of the additive manufacturing process.

While the aforementioned importance analysis methods rely on tree-based models, permutation feature importance was proposed in Altmann et al. (2010) as a broader alternative. The permutation feature importance can be used for any fitted model such as neural networks. This method is based on a simple idea that measures the decrease in the model score (e.g., coefficient of determination R^2) if the values of a feature are randomly shuffled. This approach breaks the relationship between each feature and the model output, thereby the decrease in the

model score can indicate the importance of the feature. Overall, feature importance analysis is an effective tool to enhance explainability in Mechanistic-AI. Identifying dominant mechanistic features will benefit process-structure-properties quantification and materials design in advanced manufacturing because it not only provides a smaller set of features required to be considered in the model, but also generates physical insights into the mechanisms of manufacturing processes.

3.1.2. Utilizing data invariants

Another approach to integrating physical aspects of a process into data is by exploiting the known data invariants, i.e. the aspects of data that do not influence the output. Knowing data invariants allows the development of databases that encourages AI model to be insensitive to unimportant correlations in the data which might exist due to the limited data size or biased source of information. There are generally two approaches to inform the database of such invariants: data augmentations and invariant representation.

In data augmentations, starting from a database, one can generate multiple augmented copies of the data where the copies are altered in invariant dimensions while keeping the output prediction similar to the original database. Using this method, we increase the size of the database and simultaneously encourage the machine learning model to disregard irrelevant features and correlations as it trains to accurately predict the response for original and augmented samples. The pinnacle of data augmentation is in image processing where it is a common practice to add altered versions of images to the database by applying several operations such as flipping, rotations, scaling, shearing, cropping, and varying levels of brightness and contrast.

Alternatively, we can transform the database into a representation that is inherently invariant to physically irrelevant aspects of the data. By training the machine learning model in the invariant representation space, we ensure the results of the model remain the same with changing irrelevant features of the data. A scientifically significant example of such an approach is dimensional invariance, where we can develop models that are insensitive to units and scales by representing features as dimensionless numbers. A dimensionless number is a power-law monomial of some physical quantities (Barenblatt, 2003). There is no physical dimension (such as mass, length, or energy) assigned to a dimensionless number. Using dimensionless numbers can significantly simplify the problems by reducing the number of variables that describe a physical phenomenon or process, thereby reducing the number of experiments (or simulations) required to understand and design the physical system. Furthermore, the dimensionless numbers are physically interpretable and thus provide elegant insights into the behavior of complex systems. Moreover, the dimensionless numbers do not change if the measurement system of units is changed. This allows revealing a scale-invariant relationship using small-scale experiments, which can include small length scales, small time scales, or small energy scales.

3.2. Physics-informed model development

Machine learning models are the second pillar of AI solutions. The development and training process of the ML models involve various engineering choices, which can be tuned to embed physical insights or constraints into the solution. Therefore, physics-informed model development is a key ingredient in the proposed Mechanistic-AI framework. Here, we present a collectively exhaustive categorization of approaches to embedding physical knowledge into the model development process including (1) structuring the problem into a multi-level model where different modules are developed using a combination of data-driven and physics-based models, (2) designing data-driven architectures that integrate physics in their formulation, and (3) customizing the model training process. Each category is explained in the following subsections.

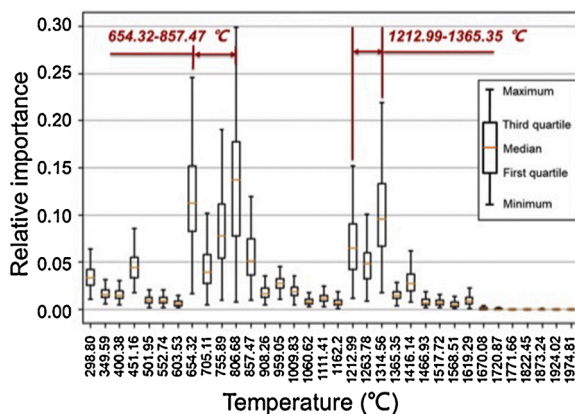


Fig. 5. Relative importance of temperature ranges in processing-induced thermal histories for ultimate tensile strength (UTS) (Xie et al., 2021).

3.2.1. Multi-level modeling

One fundamental approach to impose physics knowledge into an AI solution is by structuring the original task into submodules, where each submodule is responsible for predicting aspects of the overall model. The submodules can be structured in parallel to compensate for each other's inaccuracies or in series to break the task into simpler and more physically traceable steps. There are two main benefits to adopting this multi-level modeling method. First, the structuring of the modeling task introduces aspects of physics in the model as it enforces predicting of physically meaningful intermediate parameters. This is in contrast to the data-driven end-to-end paradigm where flexible learning comes with the cost of intermediate parameters that are, at best, very difficult to interpret. Second, this multi-level modeling approach opens many possibilities to combine physics-based modeling methods with data-driven methods. One can use physics-based modeling where reliable and efficient solutions exist and compensate them with data-driven methods. Therefore, instead of solely relying on experimental data from in-situ and ex-situ measurements and monitoring to build models, hybrid physics-based and data-driven modeling approaches can take advantage of numerical simulations to provide additional insights that cannot be easily captured through experiments. For example, maintaining constant melt pool size in AM process is important to achieve consistent properties of built parts (Gockel et al., 2014); however, it is difficult to track melt pool evolution based on experimental data alone. On the contrary, physics-based models can provide detailed information of melt pool dimensions, as deployed by Gawade et al. (2021) and Zhu et al. (2021).

An interesting example of multi-level methodology is presented by Ren et al. (2021), where a two-level data-driven model is developed to predict melt-pool size in the multi-track building of laser powder bed fusion AM. The lower-level model captures the pre-scan initial temperature for each layer and uses it as a feature in the upper-level model to predict melt-pool size. Their model achieved a lower relative mean squared error than the pure machine learning model, without the need

for a large amount of training data. Wang et al. (2020) developed a multi-level model for long-term prediction of tool wear in machining processes. Their model consists of a physics-based model and a bi-directional GRU data-driven model. The outputs of both models are passed through a dense neural network regressor to produce the final prediction, as depicted in Fig. 6. Du et al. (2021) developed a two-level physics-based and data-driven model where six simulation-based intermediate parameters of volumetric energy density, surface tension force, Marangoni number, Richardson number, pool aspect ratio, and the solidification time are initially computed using a thermal-fluid model; later, data-driven modeling is deployed to classify balling or non-balling cases in laser powder bed fusion (L-PBF). In Du et al. (2020), a steady-state computational model is used to compute temperature, strain rate, traverse force, flow stress, shear stress, and torque in friction stir welding, the outputs of the simulation is later used to predict the binary tool failure with a high accuracy of 98%.

A current limitation of multi-level modeling that combines physics-based and data-driven methods is that one needs to acquire data and train each ML model individually, which drastically increases the cost of data handling, development, and maintenance. This is because neural networks training requires access to gradients while most conventional physics-based models do not generate the gradient information. To address this challenge, a research direction has recently emerged to develop differentiable simulations, which allow a natural integration of physics-based simulation methods with neural networks. Alpha Fold (Senior et al., 2020) presented a breakthrough in solving the protein folding problem by combining a neural network model to compute a distance matrix between amino acid components with a differentiable physics-based simulation to compute the geometry of the protein. Recent studies have expanded differentiable simulations to fluid dynamics (Holl et al., 2020), computer vision simulations (Holl et al., 2020), and robotics and control applications (Qiao et al., 2020). Therefore, the extension of differentiable simulations to manufacturing applications can open new avenues in Mechanistic-AI models that

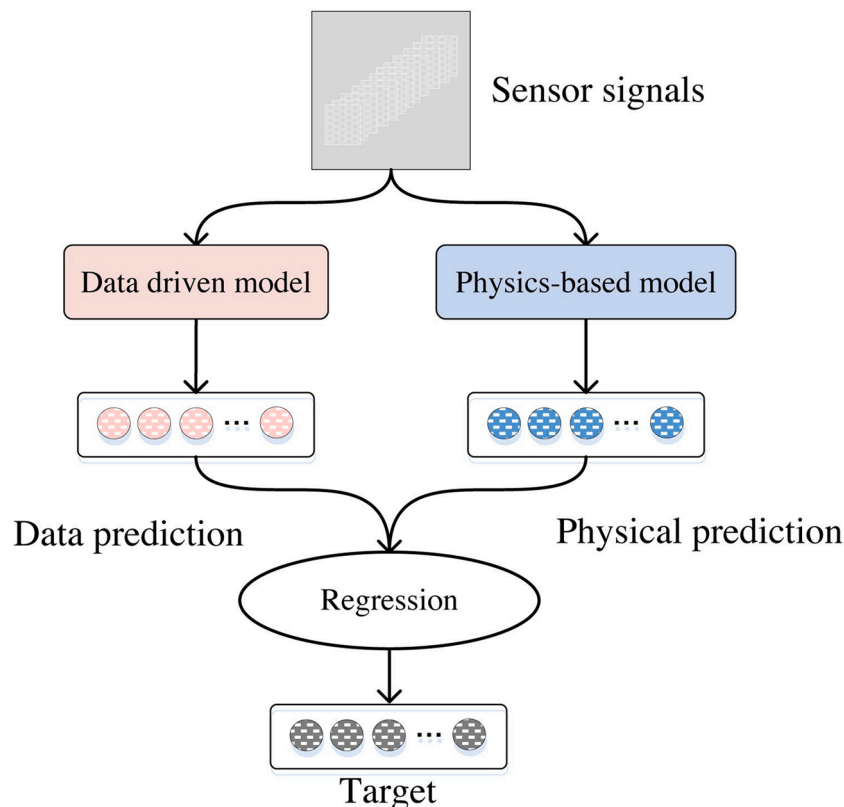


Fig. 6. A multi-level model that combines data-driven and physics-based modeling methods for tool wear prediction (Wang et al., 2020).

seamlessly integrate physics-based and data-driven approaches.

3.2.2. Model architecture design

The second approach to embed physics in data-driven model development is by developing customized formulations and architectures for machine learning models that by design uphold certain physical attributes. Some of the most popular neural networks (e.g., CNN, RNN, attention mechanism) belong to this class. CNNs inherently process neighboring information by passing a local kernel through the image. RNNs (e.g., LSTM and GRU) are designed to pass long-term correlations for an arbitrary number of time-steps without saturating the gradient information through gated mechanisms. Arguably, one of the main reasons behind the explosive adoption of neural networks is the flexibility and scalability of their formulation that allows creating a wide range of architectures for different applications. Introducing novel architectures is an extremely active research field with every year numerous new formulations and architectures are developed inspired by biology (Hasani et al., 2020), physics (Owhadi and Yoo, 2019), or heuristics of the task at hand (Cohen et al., 2019). For example, inspired by biology, Hasani et al. (2020) developed a neural network formulation that incorporates an abstraction of synapse interactions in neurons. Their model is a neural ordinary differential equation (neural ODE) architecture that incorporates conductance-based synapse formulations. The authors show that they can perform time-series prediction with higher stability and expressivity compared to conventional recurrent neural networks.

In the manufacturing field, Mozaffar et al. (2021) presented a model of AM thermal responses such that it generalizes to unseen complex geometries. To achieve this, they developed a customized neural network architecture that computes mesh-level dependencies inspired by finite element calculations and aggregates neighboring interactions to capture long-term evolution of thermal responses given the

manufacturing process parameters such as laser power, toolpath, and material properties. The architecture consists of graph neural networks for mesh-based computations and recurrent neural network for time series analysis, as depicted in Fig. 7. Zhang et al. (2020) developed a recurrent neural network-based architecture which is augmented by an attention mechanism to predict the tensile strength in fused deposition modeling (FDM) processes. In their architecture, they exploit the layered nature of AM processes and correspond each layer to one LSTM cell to extract the relative influence of each layer on the final part behavior. Saha et al. (2021) developed a new architecture, called HiDeNN, that defines the weights and bias as functions of nodal positions and is designed to find the optimal nodal positions by minimizing the potential energy of mechanics problems. They embedded a scaling network into a neural network to automatically discover dimensionless numbers from experimental data, which is later passed through a dense neural network layer to predict final parameters of interest (see proposed architecture in Fig. 8). This method is applied in a fluid mechanics problem and recovered Reynolds number Re and relative surface roughness Ra^* . Note that this method is currently limited to predicting dimensionless outputs and it can be impractical to determine the number of dimensionless parameters in many complex systems, which can be a worthwhile topic for future improvements.

Another promising example is the AI-coupled crystal plasticity-based modeling techniques, which is one of the virtual material characterization methods that have been widely utilized to facilitate the research and development of new materials and manufacturing methods. Ali et al. (2019) used a fully connected neural network model coupled with a rate-dependent crystal plasticity finite element method formulation to predict the stress-strain and texture evolution of AA6063-T6. The run-time comparison test shows that the developed model saves more than 99.9% of the computational time compared to the conventional crystal plastic model. Ibragimova et al. (2021) designed a framework where an

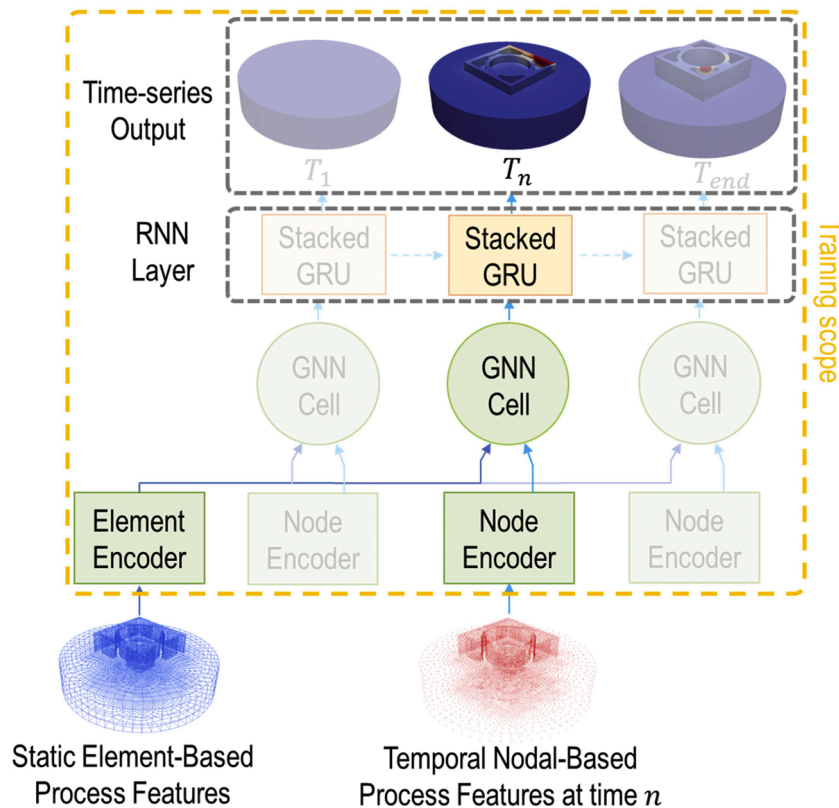


Fig. 7. A customized neural network architecture which uses mesh-level elemental and nodal features to compute local geometry-dependent interactions for thermal modeling of AM processes. The network receives manufacturing process parameters as local features and predicts evolution of thermal responses over an arbitrary number of time steps (Mozaffar et al., 2021).

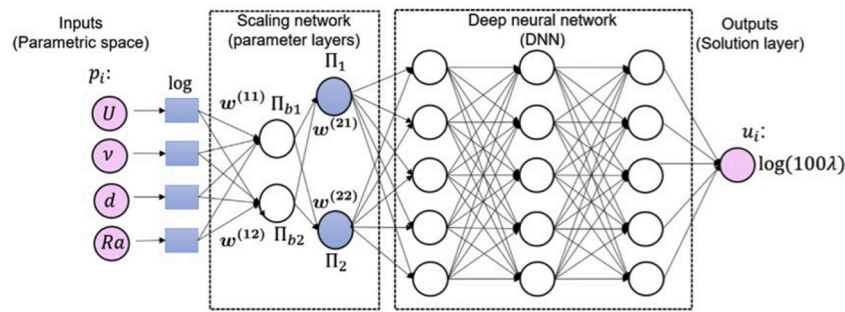


Fig. 8. A customized neural network architecture which embeds a constraint of physical dimensions of different input parameters in network design (Saha et al., 2021).

ensemble of fully connected neural networks are trained with the dataset generated from crystal plasticity simulations to model stress-strain and texture evolution for face-centered cubic (FCC) family crystals under a non-monotonic strain path. Each neural network in the ensemble was used to predict a component of the output variables separately and a comparison test was performed to design the architecture of the network for each variable. The results show that the model predicts the stress with an average error of less than 10 MPa and the texture evaluation less than 1A°.

3.2.3. Customized model training

The third approach to integrating physical knowledge into data-driven modeling is by customizing their training process. A prominent research direction in this line is introduced by Raissi et al. (2017) in which an additional loss function based on the residuals of physical conservation laws is incorporated into regular neural network loss in order to guide the training process of neural networks. This method of customized training by augmenting the loss function is named as physics-informed neural network (PINN) (Raissi et al., 2017). There are two main advantages for PINNs: (1) it can seamlessly combine experimental data with partially or fully understood physics-based models, which means that model predictions can fit physical laws and experiments at the same time (2) it only needs space and time coordinates as inputs and does not require the corresponding output like velocity, pressure, or temperature field because it optimizes model parameters by minimizing a loss function including governing equations. That is to say, unlike classical ML approaches, it does not need to prepare a training set before training.

Specifically, PINNs are designed to find the mapping from co-ordinates to a partial differential equations (PDEs) solution using feed-forward neural networks. Based on automatic differentiation in PyTorch or Tensorflow, we can easily compute derivatives with different terms in PDEs and then obtain the residuals of conservation laws. Experimental data prediction error can also be added in the loss function as a soft penalty. Therefore, the general form of the loss function can be written as:

$$\text{Loss} = \lambda_1 \text{MSE}_{\text{PDE}} + \lambda_2 \text{MSE}_{\text{data}} \quad (1)$$

where MSE_{PDE} is the error that encourages lower residuals of PDEs on sampled coordinates and MSE_{data} is the error of the approximation $u(x, t)$ at known data points. λ_1 and λ_2 determine the importance of MSE_{PDE} and MSE_{data} , respectively. Note that several variations of PINNs are proposed for static, continuous dynamics, and discrete-time dynamics problems. For example, in a continuous-time network, one can consider coordinate x and time t as inputs and uniformly sample them inside the time and space domain, while for a discrete-time network, one can consider coordinate x as the input and the unrolled solution of u^i ($i = 1, 2, \dots, n$) as the output.

PINNs have achieved promising results in fluid mechanics (e.g., Jin et al., 2021; Cai et al., 2021), biology (e.g., Yin et al., 2021; Arzani et al.,

2021), and environmental study (e.g., He et al., 2019). However, only a few studies have attempted to deploy PINNs in manufacturing applications. Zhu et al. (2021) applied PINNs in three-dimensional additive manufacturing (AM) process modeling to predict temperature field and melt pool dynamics with a moderate number of data points. They imposed the Dirichlet boundary conditions using a Heaviside function instead of a soft penalty in the loss function to accelerate the training process. The input of the network includes AM parameters, material properties, and location of interests, and the outputs are the corresponding temperature and melt pool velocities. Their model is validated on 2018 NIST AM-Benchmark test data and reveals the potential for PINNs in advanced manufacturing.

Apart from modifying the loss function, one can develop a customized curriculum for the training process in a transfer learning scheme. Researchers studied methods to pre-train a surrogate model with a large amount of simulated data and then fine-tune the model with a smaller number of experimental data, (e.g., Jha et al., 2019; Moges et al., 2021). The motivation behind this method is to take advantage of both experimental data and simulated data while avoiding the drawbacks of each data type, i.e., limited accuracy of simulation data and limited availability of experiments. Jha et al. (2019) developed a deep transfer learning approach to achieve robust material property prediction, which is shown in Fig. 9. They first pre-trained a data-driven model with a large computational dataset (about 341 K samples) and later trained the model with a small set of experimental data. They showed that compared to training a model from scratch, transfer learning achieves lower prediction error.

Moges et al. (2021) developed a hybrid modeling framework that integrates physics-based data with measurement data to predict melt-pool width in laser powder bed fusion processes. They generated a set of melt pool data with different process conditions using a high-fidelity CFD model and collected experimental data from ex-situ melt pool optical images with similar process parameters. To build a hybrid model, they first trained a surrogate model based on simulation data using polynomial regression. They further train their model to minimize the residual error in experiment results using unbiased adaptive sampling between simulation and experimental data, which led to more accurate model compared to the physics-based simulations. The schematic of their hybrid modeling approach is shown in Fig. 10.

Interestingly, Kapusuzoglu and Mahadevan (2020) studied three variations of physics-informed model development approaches mentioned in this section for fused filament fabrication (FFF) processes. Their simulated data came from a sequential multiphysics model (thermal model and polymer sintering model) which can generate a dataset about porosity and bond quality under different process conditions. They included a small number of experimental data and studied eight separate hybrid modeling methods in three categories. Their results show that incorporating physical constraints in the loss function enables the model to produce the most physically consistent results, while the multi-level modeling and hybrid training methods lead to suboptimal results.

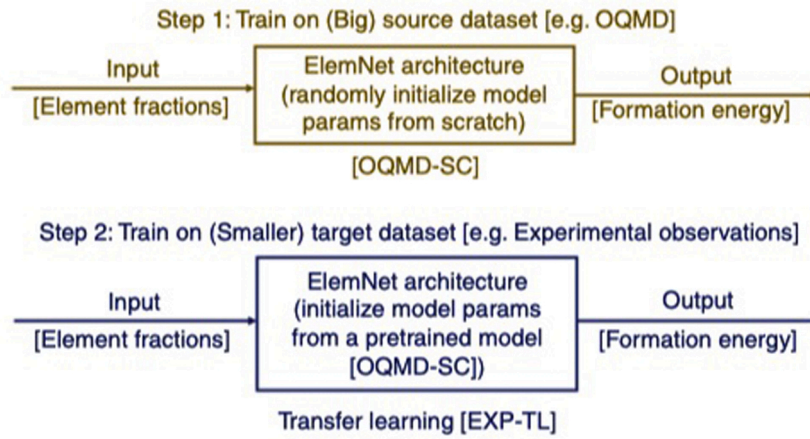


Fig. 9. Deep transfer learning of material property prediction by training from large computational datasets (such as Open Quantum Materials Database (OQMD)) and fine-tune the model with a small number of measurement data (Jha et al., 2019).

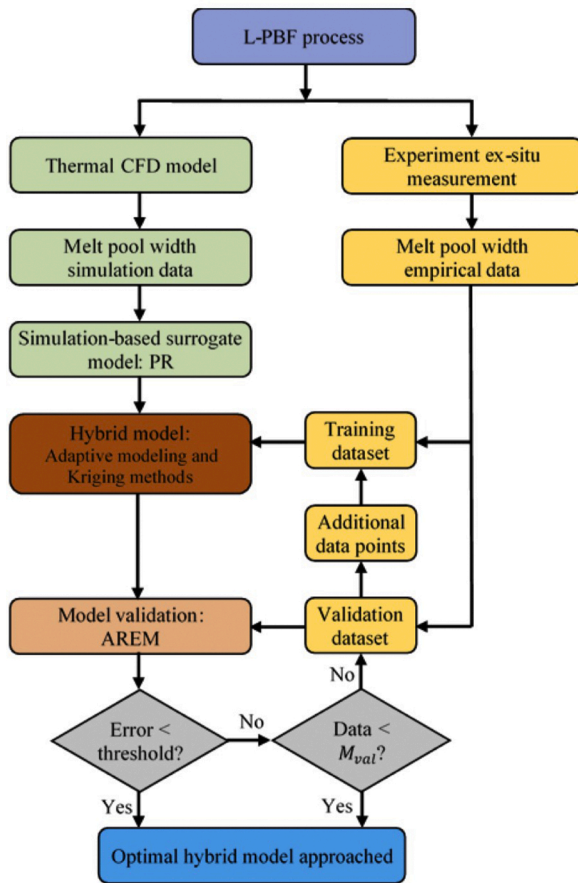


Fig. 10. Workflow for hybrid modeling approach to predict melt-pool width in laser powder bed fusion processes (Moges et al., 2021).

Finally, despite the progress and advantages of customized modeling development methods, such as PINNs, currently there are important limitations to these approaches: (1) many complex system does not have a closed form of governing Eq. (2) experimental data is usually scarce and noisy and how to combine low-fidelity with high-fidelity is still an open question; and (3) the optimization and network design require trial and error with many hyperparameters.

3.3. Data-driven discovery in manufacturing

Most of the advanced manufacturing processes have multiphysics and multiscale nature, in which we know some physics while missing some information about boundary conditions and governing equations (Karniadakis et al., 2021). For example, in laser-based manufacturing, high energy laser beam interacts with a substrate material, which could lead to intensive vaporization of the melted material (Gan et al., 2021). We still do not fully understand the complex interactions between laser, liquid material, vapor plume, and possible laser-induced plasma. Despite the progress in the development of models to quantify the complex manufacturing processes and match the experimental measurements, this development process can be tedious and time-consuming, involving proposing a hypothesis, examining model assumptions, selecting appropriate equations and boundary conditions, and developing numerical methods to solve the problems. In addition, sophisticated calibration techniques are required for tuning unknown parameters in the models.

Recent advances in machine learning and AI have introduced an alternative methodology, called data-driven discovery, which promises to discover governing equations and underlying properties of a system directly from collected data. This new methodology can significantly accelerate the quantification of the hidden physical mechanisms and interactions underlying the manufacturing processing. The identified compact equations or laws could enable efficient process and materials design in advanced manufacturing. In this section, we review several rapidly evolving methods for discovering (1) differential equations and (2) dimensionless scaling laws from data. Furthermore, we discuss how to apply those mathematical methods to advanced manufacturing fields.

3.3.1. Data-driven discovery of differential equations

A milestone in the field of data-driven discovery of differential equations is the sparse identification of nonlinear dynamics (SINDy) proposed by Brunton et al. (2016). It was inspired by an earlier work (Schmidt and Lipson, 2009) on extracting hidden equations of a nonlinear dynamical system from data using symbolic regression (Koza, 1992). SINDy is a machine learning algorithm that extracts dynamical systems, described by ordinary differential equations (ODEs) or partial differential equations (PDEs), from collected data. Time-series data can be used for discovering ODEs as expressed in Eq. (2), where $\mathbf{x}$ is the state variables evolving in time t needed to describe the system and $f(\cdot)$ is an unknown function to be identified from data. Spatio-temporal data are required to discover PDEs as expressed in Eq. (3), where $\mathbf{u}$ is a spatio-temporal field evolving in space and time.

$$\frac{d}{dt}x = f(x) \quad (2)$$

$$\frac{\partial}{\partial t}u = N(u) \quad (3)$$

Given a set of time-series data or spatio-temporal field data, SINDy aims to discover a sparse set of governing equations out of a pre-defined pool of possible mathematical forms that could describe the data. SINDy can identify ODE or PDE equations that are sparse and have as few degrees of freedom as possible, similar to the Lorenz equations or Navier-Stokes (N-S) equations. This is in contrast with most modern over-parameterized machine learning methods, such as neural networks.

A schematic of the SINDy algorithm is illustrated in Fig. 11 using a simple example of a Lorenz system. Assuming that we only have access to observed data from the Lorenz system (i.e., measurements of the state x , y , and z in time). One can arrange this data into a matrix $\mathbf{X}$, where every row of $\mathbf{X}$ is a measurement in time. We can also compute the state derivatives $\dot{x}$, $\dot{y}$, and $\dot{z}$ using numerical methods (e.g., finite differences or Total Variational Derivative Chartrand, 2011), and similarly arrange them into a matrix $\dot{\mathbf{X}}$. In the SINDy method, we create a library matrix that consists of all possible terms that describe the dynamics of the system, starting with linear terms and gradually expanding to nonlinear expressions. For example, the library matrix $\Theta(\mathbf{X})$ can consist of x , y and z , as well as nonlinear terms x^2 , xy , xz , y^2 and up to the fifth-order polynomials. Ideally, we want our library $\Theta(\mathbf{X})$ to include all dominant terms that are required to describe the left-hand side derivatives $\dot{x}$, $\dot{y}$, and $\dot{z}$. It is noted that the terms in the library (gray columns in Fig. 11) $\Theta(\mathbf{X})$ can be computed from the measured data x , y , and z . Now, the problem is reduced to a sparse optimization problem with the objective to find the fewest terms in this library of candidate dynamics $\Theta(\mathbf{X})$ that best describe the time derivatives $\dot{\mathbf{X}}$. Several sparse optimization algorithms can be deployed to find the sparse coefficient matrix Ξ . Examples of the sparse optimization algorithms include lasso (Tibshirani, 1996) (i.e., linear regression with L-1 norm regularization) and sequential threshold least-squares (STLS) (Brunton et al., 2016). Finally, one can use the selected terms in $\Theta(\mathbf{X})$ and corresponding coefficients in Ξ to reconstruct a minimalistic model of the dynamical system. In this case, the authors showed that they can recover the complete form of the Lorenz equations.

Compared to the traditional methods, such as brute force search

(Korf, 1999) and the genetic programming method (Schmidt and Lipson, 2009), the SINDy algorithm is more efficient and scalable (Kaheman et al., 2020). Although the dynamical equations are assumed to be linear combinations of nonlinear candidate terms in the library, this assumption is reasonably valid for many engineering dynamical systems. Many improvements and extensions are proposed to the SINDy algorithm to discover PDEs (Rudy et al., 2017), identify dominant coordinate systems (Champion et al., 2019), and handle with time-varying coefficients (Li et al., 2019a). Importantly, the identification of multiscale models for anisotropic material responses is studied in Brunton and Kutz (2019). Fortunately, these methods are widely available for researchers as the authors released an open-source Python library of the algorithms, Pysindy (de Silva et al., 2020), and Steven Brunton, the first author of the SINDy paper, has made a series of well-made tutorial videos on YouTube (Brunton, 2021).

Recently, the SINDy algorithm and its variants have been applied in several sciences and engineering fields, including fluid mechanics (Brunton et al., 2020b), biology (Mangan et al., 2016), system control (Kaiser et al., 2018), materials chemistry (Bartel et al., 2018), aerospace engineering (Brunton et al., 2020a), and magnetohydrodynamics (Kaptanoglu et al., 2020). However, very few people successfully apply the SINDy or other data-driven discovery methods to advanced manufacturing fields and address the unique challenges of this interdisciplinary research. Note that the accuracy of the identified equations and expressions highly depends on the data quality. In-situ, high-speed, high-resolution measurement data is invaluable for the data-driven discovery of manufacturing processes. To discover experimentally-validated dynamical systems (i.e., governing ODEs and PDEs) underlying the manufacturing processes, in-situ measurements including time series (e.g., temperature series in time) or spatio-temporal fields (e.g., strain fields in space and time) data are required. Examples of in-situ measurements that are appropriate to be analyzed using the SINDy algorithm include high-speed photography (Chen et al., 2013), infrared thermography (Yang et al., 2017), synchrotron X-ray imaging (Zhao et al., 2017), X-ray computed tomographic (CT) (Thompson et al., 2016), in-situ X-ray Diffraction (XRD) (Oh et al., 2021), particle image velocimetry (PIV) (Ho et al., 2020), and digital image correlation (DIC) (Xie et al., 2019).

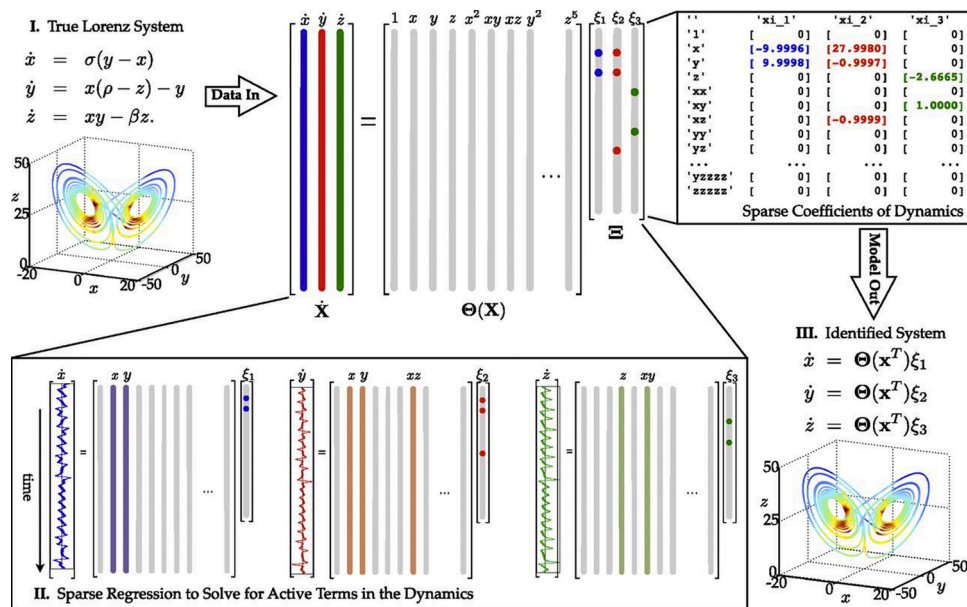


Fig. 11. Schematic of the SINDy algorithm using an example of the Lorenz equations (Brunton et al., 2016). It includes three parts: (I) true Lorenz system used for data generation, (II) sparse regression to solve for active terms in the dynamics, and (III) identified system.

3.3.2. Data-driven discovery of dimensionless scaling laws

Dimensionless numbers and the relationships between them, i.e., dimensionless scaling laws, play a critical role in scientific fields. More than 1200 dimensionless numbers have been discovered in an extremely wide range of fields, including physics and chemistry, fluid and solid mechanics, thermodynamics, electromagnetism, geophysics and ecology, and various engineering disciplines (Kunes, 2012). In advanced manufacturing, much effort has been directed at identifying process- and material-related dimensionless numbers and scaling laws to simplify the highly multivariable manufacturing processes with multiple interacting physical phenomena. Some of the dimensionless scaling laws are claimed to be “universal”, which apply broadly and remain accurate for different materials, processing conditions, even manufacturing processes. For example, a recent study identified a universal dimensionless scaling law for laser-induced vapor depression morphology (i.e., keyhole aspect ratio) (Gan et al., 2021) as shown in Fig. 12.

Many scaling laws are provided in the field of advanced manufacturing and have been validated by experimental data. The predicted manufacturing variables include relative density of fabricated parts (Rankouhi et al., 2021), lack-of-fusion porosity (Gan et al., 2021), laser-induced melt pool geometries (Yang et al., 2021), laser absorptivity (Ye et al., 2019), keyhole geometries (Wang and Liu, 2019), keyhole porosity (Gan et al., 2021), hot tearing susceptibility (Monroe and Beckermann, 2014), dimensionalless cooling rate (Bontha et al., 2006), and dimensionless thermal strain parameter (Knapp et al., 2017). Most of the mentioned dimensionless numbers and scaling laws are identified using dimensional analysis (Tan, 2011), which carefully examines the units of the physical systems to identify a set of dimensionless numbers that constitute the essential and scale-invariant physical relationships (Jofre et al., 2020). However, the classical dimensional analysis based on Buckingham π theorem (Buckingham, 1914) has two well-known limitations: (1) the derived dimensionless numbers are not unique, and (2) the relation between dimensionless numbers (i.e., scaling law) remains unknown for general cases, and thus it is impossible to measure the relative importance of the dimensionless numbers or identify a dominant set of dimensionless numbers. Therefore, the conventional approach can be time-consuming as it requires multiple trial and error iterations.

The classical dimensional analysis can be complemented by advanced data science and AI, i.e., data-driven dimensional analysis (Constantine et al., 2017). This methodology provides a systematic way to integrate data science and dimensional analysis and overcome the limitations of the classical dimensional analysis and discover high-quality universal dimensionless scaling laws from data. Mendez and Ordonez (2005) proposed an algorithm called SLAW (i.e., Scaling LAws) to identify the form of a power law from experimental data (or

simulation data). The proposed SLAW combines dimensional analysis with multivariate linear regressions. This approach has been applied to some engineering areas, such as ceramic-to-metal joining (Mendez and Ordonez, 2005) and plasma confinement in Tokamaks (Murari et al., 2015). This algorithm assumes the relationship between the dimensionless numbers obeys a power law, which is invalid in many applications. For example, the relationship between friction factor and Reynolds number in the turbulent regime of the pipe flow dynamics is not a power law. Constantine et al. (2016) proposed a rigorous mathematical framework to estimate unique and relevant dimensionless groups. Active subspace methods are connected to dimensional analysis, which reveals that all physical laws are ridge functions (Constantine et al., 2016). They demonstrated their algorithms using both laminar and turbulent viscous pipe flow examples. Their method is applicable to idealized physical systems meaning that (1) the experiments can be conducted for arbitrary values of the independent input variables (or dependent input variables with a known probability density function), and (2) noises or errors in the input and output are negligible. Saha et al. (2021) proposed a Hierarchical Deep Learning Neural Network (HiDeNN) to combine deep learning and dimensional analysis to discover dimensionless numbers from experimental data. This method is recently generalized as a methodology, called dimensionless learning (Xie et al., 2021), in which the principle of dimensional invariance is embedded in machine learning to automatically discover dominant dimensionless numbers and scaling laws from data. The proposed approach has been demonstrated using noisy experimental data collected from a wide range of problems including turbulent Rayleigh-Benard convection, vapor depression dynamics, and porosity formation in additive manufacturing.

Data-driven dimensional analysis is still an active field. Much effort is required to improve the efficiency, interpretability, predictivity, and robustness of the algorithms. Using the developed algorithms to explore high-quality manufacturing data, many universal dimensionless numbers and scaling laws are expected to be discovered, which can provide elegant insights for manufacturing process optimization, defects elimination, new materials development, and mechanical performances improvement.

4. AI in manufacturing design

In design tasks, we attempt to identify the process of building a part that meets a set of requirements. Design in manufacturing has traditionally been studied in two separate steps: (1) conceptual design and (2) process design. The conceptual design step refers to the envisioning of the geometric parts and materials. In practice, the conceptualization step is a mostly deterministic process that is performed using computer-

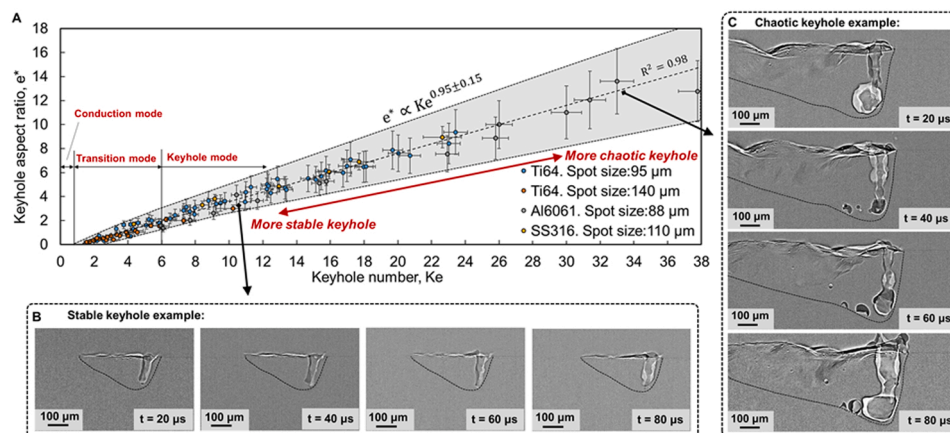


Fig. 12. A scaling law for keyhole aspect ratio controlled by the Keyhole number, a dimensionless number combining seven process parameters and material properties (Gan et al., 2021).

aided design (CAD) software. The process design step, on the other hand, realizes a manufacturing setting to achieve the developed conceptual design. Process design involves several steps including manufacturing process selection, process parameters optimization, and system-level optimization given machine availability, supply chain, and maintenance—often developed using computer-aided manufacturing (CAM) and computer-aided process planning (CAPP) tools. The optimality of the design involves multiple competing factors such as quality of the part under various performance metrics (e.g., strength, geometric accuracy, thermal behavior), cost, production rate, and the robustness of the solution to defects and disturbances.

Design has remained one of the core engineering and scientific pursuits due to several challenging aspects of the process. The information involved in the design process is often unstructured, high-dimensional, noisy, and sparse; thus, making the mapping between requirements and design difficult to discover. Manufacturing involves many discrete choices and nonlinear constraints, which generates poor-conditioned optimization settings. Additionally, there is a nontrivial level of uncertainty in the design process (e.g., due to machine-specific behavior, discrepancies in modeling tools, and unknown material characteristics) that make the process stochastic. Therefore, the design process requires years of experience to efficiently produce reliable parts and involves tedious and expensive rounds of trial and error.

Traditionally, designers use Design for Manufacturing (DFM) guidelines to reduce the complexity of the design process. These guidelines are based on rough characteristics of the design geometric components and lack the complexity to adequately analyze complex designs. Additionally, existing DFM does not offer a unifying set of principles for manufacturing processes; rather, the rules are vastly different for each process. For example, several studies developed guidelines that are only applicable to specific types of metal-based AM processes (e.g., Kranz et al., 2015; Walton and Moztarzadeh, 2017). Therefore, a design engineer needs to make critical decisions about the manufacturing process as early as conceptualization in order to use such DFM tools, which makes various tasks within conceptual and process design highly intertwined. Other conventional attempts to automate the design process build upon detection systems with manually engineered geometric features (e.g., Han et al., 2000; Kazhdan et al., 2004) or sophisticated manufacturing ontologies (e.g., Jang et al., 2008; Dinar and Rosen, 2017), both of which are difficult to adapt and scale to new processes as they heavily rely on expert knowledge. In this section, we advocate for novel AI solutions in manufacturing design problems as AI provides a unique capability to explore massive design spaces and complex interactions common in manufacturing processes. We look for design methods that offer better performance than the conventional approaches or reduce the number of steps in the design process by

integrating multiple tasks, as shown in Fig. 13.

We categorize publications on AI in manufacturing design into two classes of (1) direct mapping of functional requirements to design parameters, and (2) inverse design optimization. Noteworthy developments and successful examples in each category are elaborated upon in the following subsections with a focus on methods to incorporating physical mechanisms and constraints of manufacturing processes into AI formulations. Note that while modeling methods can greatly facilitate in design tasks, as we discussed modeling advances in Section 3, here, we exclude those contributions.

4.1. Direct mapping for design

As the ultimate goal of design is to find optimal design parameters given functional requirements, a natural approach is to directly map requirements to parameters. This is particularly a compatible concept with modern deep learning methods since they are known for extracting complex and unsuspected correlations between various data structures. Therefore, several compelling research areas have recently emerged that fit into this design category. A popular approach to analyze manufacturing and material systems is to hierarchically model the relationships between the manufacturing process parameters, material structure, properties, and performances (PSPP) (Olson, 1997). Therefore, AI can be used to model any of such causal relationships in the reverse direction, producing a design tool.

Jiang et al. (2020) took a supervised learning approach to directly map the strain-stress response curve to the design parameters of unit structures geometries in a polymer jetting process. They used the data extracted from 300 parts to train a fully connected neural network that predicts the desired design of unit structures in a customized ankle brace design. Their design framework with reverse PSPP connections is depicted in Fig. 14. Hashimoto and Nakamoto (2021) used machine learning to design the process plan for machining processes. The authors developed a U-net architecture performing voxel-wise segmentation on 243 3D geometries, which is labeled according to past machining processes performed by skilled experts. The inputs and outputs of the network are one-hot encoded and include the voxel geometry, accuracy measures (with two states for low and high accuracy requirements), cutting tool type (with two states for ball and flat endmills), and toolpath pattern (with three states for contour line, scanning-line, and along-surface patterns). In a hierarchical decision-making process, first, the voxel-wise cutting tool type is predicted given the geometry and required accuracy. Later, the cutting tool type is used along with other inputs to decide the toolpath pattern. The voxel-wise predictions are aggregated using a majority voting method to produce the final decision for each major machining surface. Zhao et al. (2020) proposed a

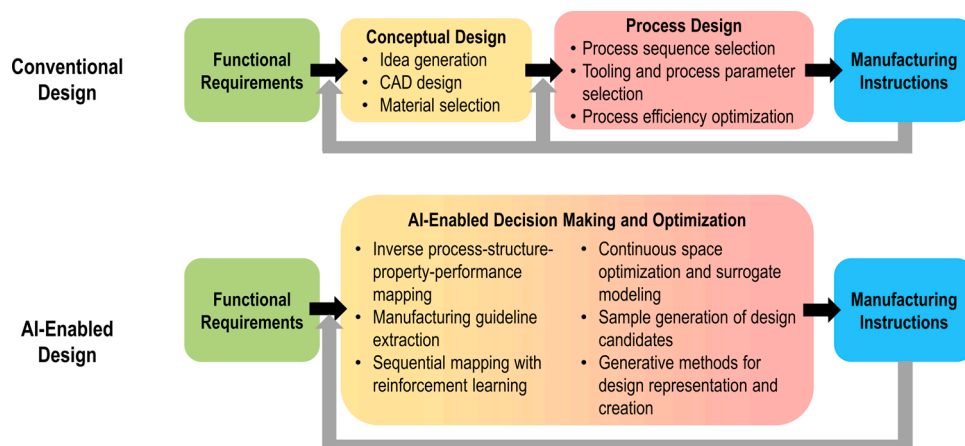


Fig. 13. Design in conventional design includes several disconnected steps in conceptual design and process design (top). AI-enabled design methods that aim to autonomously optimize the design process and integrate several design tasks (bottom).

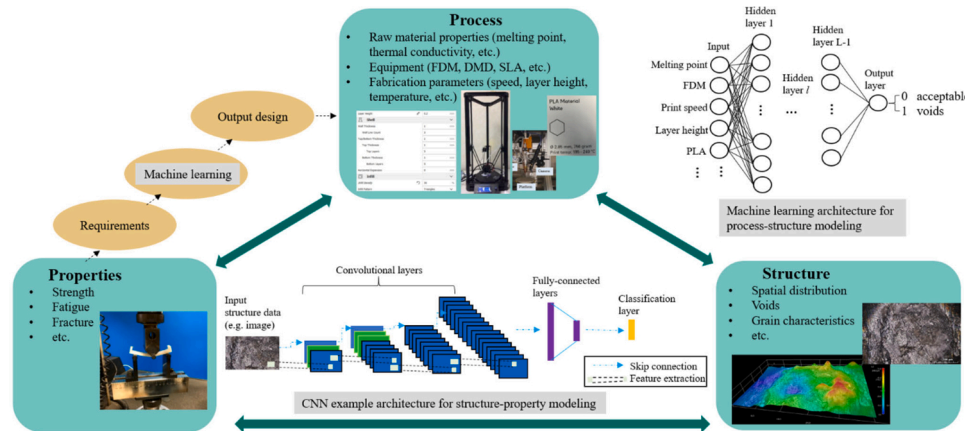


Fig. 14. Conventional process-structure-property (PSP) modeling establishes a causal link between manufacturing and material parameters. Using ML, each link within the PSP relationships can be modeled in the reverse direction to produce a design tool. For instance, the desired mechanical properties can be linked to required microstructure descriptors (Jiang et al., 2020).

data-driven method to select a manufacturing process between milling, turning, and casting based on shape, quality, and material properties. They compute a histogram based on various attributes of the CAD geometry, including curvatures distribution, rotational symmetry, and pairwise surface point distances. The geometric descriptors along with material properties (e.g., yield strength, Young's modulus, thermal conductivity) and quality attributes (global surface roughness and tolerance) are fed into decision-tree classifiers and trained to achieve an accuracy of 88% on complex geometries while training on 81 parts.

As another intriguing application of supervised learning in design, recent studies explored the capability of machine learning to better extract automated guidelines for manufacturing processes. Williams et al. (2019) developed a deep learning model to evaluate the manufacturability of additively manufactured parts. Their model, trained over 72,000 synthetic samples, receives voxelized CAD geometries, and generates manufacturing metrics such as support mass and build time. Guo et al. (2021) assessed the manufacturability of metal cellular structures in the direct metal laser sintering process, where parts with severe warpage due to residual stress, cracking, and delamination are classified as non-printable. This research trains a hierarchical autoencoder to extract dense features of the voxelized geometries. Furthermore, to effectively train a convolutional neural network classifier based on limited experimental data, they proposed a semi-supervised method, in which a generative adversarial network is trained to differentiate between labeled experimental data, unlabeled experimental data, and synthesized data; hence, forcing the network to maximally utilize valuable experimental data. Zhang et al. (2018) trained a network with 3D convolutional layers to recognize machining features in the voxelized space. The model is trained over 144,000 geometries using an incremental learning approach and achieves an accuracy of 97%. To assist the conceptual design process, Kwon et al. (2021) developed a multi-modal search to retrieve inspirational 3D design examples based on text keywords, geometric appearance, and functional similarities. Using a neural network-based architecture and contrastive learning, they extract embeddings of text and visual queries, in which parts with similar attributes map to close embeddings in the design latent space. For new search inquiries, the new embedding values are extracted and the database sample closest to them in the embedding space is retrieved.

There is a key drawback in the existing supervised methods for design. Manufacturing processes commonly involve many constraints that limit the feasible space of design parameters, performances, as well as the path to reach them. The correlational direct mapping methods in the literature disregard such constraints and, therefore, can easily lead to unfeasible solutions. This is particularly challenging as many of such constraints are complex and cannot be easily formalized. Reinforcement

Learning (RL) offers a plausible solution to this problem. In RL an agent can learn to optimize an arbitrary reward function by exploring the design space. By shaping the rewards in a way that we penalize constraint violations, the agent can implicitly learn about the constraints of the design space and avoid unfeasible solutions. RL methods are well-suited in applications with a sequential decision-making nature as they exploit the temporal aspects of the agent interactions and identify the influence of individual actions on the final performance (known as the credit assignment problem). Dornheim et al. (2021) developed an RL agent that finds multi-step processing paths to reach the desired microstructure in metal forming processes (see Fig. 15). The state representation is defined as a transformation of orientation distribution function (ODF) using generalized spherical harmonics. This transformation considers the symmetry conditions in microstructures and thus allows for a more condensed representation. To avoid sparsity in the reward structure, they introduce a potential-based dense reward function based on the distance between the current and target microstructural patterns. They deploy a model-free agent, based on the deep Q network (DQN) formulation, to dynamically adjust the displacement of the die in the process with the aim to find a path from an initial structure to one of the equivalent target structures. Interestingly, the proposed RL framework learns the most achievable target structure by the agent along with the path to process path to reach it.

Mozaffar et al. (2020) utilized the RL framework for the tool path design task in additive manufacturing. They build upon three predominant RL algorithms, namely DQN, PPO, and SAC, to design tool paths for arbitrary section geometries in a pixelized space and showed that RL methods can surpass the performance of engineered zig-zag toolpath strategies common in industrial practices when defining a dense reward structure is possible. However, they point out that model-free RL algorithms struggle in scenarios with sparse rewards. Lee et al. (2019) investigated the performance of a variation of the DQN method, double deep Q-network, in engineering design of microfluidic devices. In their papers, the RL agent designs the location of several micro-pillars to achieve an arbitrary desired flow pattern in pixel space. They deploy a reward-shaping strategy that provides small rewards encouraging the agent to approach the goal and a large reward for finding acceptable solutions. Additionally, they demonstrate that the trained agent can be fine-tuned to outside of training problems (e.g., different numbers of micro-pillars) with minimal refinement training.

4.2. Inverse design optimization

Another approach to design in manufacturing is to follow the causality link that produces the performance and formulate it as an

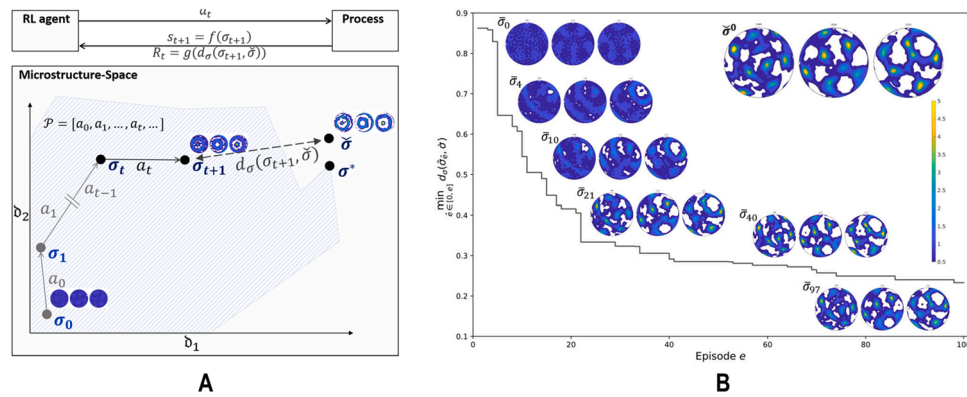


Fig. 15. Reinforcement learning agent finds a manufacturing path in the microstructure space to reach an equivalent target structure (A). Evolution of the designed microstructures during the training process (B) (Dornheim et al., 2021).

optimization problem where one iteratively modifies the design parameters to minimize an objective function related to the part performance. Many have adopted and applied PSPP as a framework to model material evolution in manufacturing processes. However, as the formulations for linking part behaviors are rarely differentiable, gradient-based optimization tools are not readily applicable. Additionally, gradient-free methods can be computationally expensive as they scale poorly to high-dimensional problems. A well-established practice is to develop surrogate models on top of the physics-based simulation tools to provide inexpensive access to gradients and perform the optimization in the surrogate space. Shahan and Seepersad (2012) developed such a surrogate model using a Bayesian network classifier to improve the design of unmanned aerial vehicles. A similar method is used in Matthews et al. (2016) to optimize the stiffness of metamaterials. Pacheco et al. (2003) proposed a multi-stage Bayesian surrogate in a thermal design problem.

Recently, the same philosophy is combined with modern machine learning and optimization methods. Tang et al. (2021) developed a method to design an AM-built shoe sole with minimum pressure points while simultaneously adjusting the overall geometry and porous structure. They divide the part into sub-regions to allow applying different patterns in sensitive areas. A Gaussian Process Regression is trained to predict the parametrized lattice behavior using 40 simulation samples, and a sequential linear programming optimizer is deployed to find parameters leading to a decreased level of pressure points. Finally, they compile the proposed design by connecting sub-region lattice structures. Mohamed et al. (2021) optimized the dimensional accuracy of cylindrical parts in fused deposition modeling processes. They used a second-order definitive screening design method to generate a design of experiment space, capturing 99% of the variation in the response with a small number of samples, train a fully connected neural network, and optimize the process on the developed surrogate model.

While arguable a less popular approach since the rise of the neural networks, evolutionary-based optimization methods have also been studied for the manufacturing design tasks in the literature. Ghosh and Martinsen (2020) deployed and benchmarked various evolutionary optimization methods, including Non-Dominated Sorting Genetic Algorithm (NSGA-III) and Multi-Objective Evolutionary Algorithm based on Decomposition (MOEA/D) for process design in manufacturing. They demonstrated that using a Gaussian kernel regression surrogate model, they can optimize 11 different manufacturing design tasks in the literature involving turning, grinding, heat exchanger tube, milling, abrasive water jet machining, dry turning, drilling, welding, and emulsification processes. A similar concept is demonstrated in other manufacturing design tasks by Abbas et al. (2020) and Vukelic et al. (2021).

Differentiable physics-based approach (Hu et al., 2019), as discussed in Section 3.2.1, is an alternative to surrogate modeling. In differentiable simulations, the gradients of an arbitrary computational path can be

efficiently computed using the automatic differentiation (AD) formulation. This enables high-dimensional gradient-based optimization without the need for surrogate modeling and provides natural integration with neural networks which can be particularly helpful in design tasks. An example of this approach in manufacturing is presented by Mozaffar and Cao (2021) where a differentiable simulation for thermal analysis of additive manufacturing and demonstrated that the physics-based simulation combined with neural networks can design time-series laser power to achieve desired thermal and melt pool behavior.

Instead of optimizing toward a single design, many design applications can benefit from methods that generate multiple promising candidates. Paul et al. (2019) developed a method that designs a spectrum of microstructures with optimized thermal expansion, stiffness coefficient, and yield stress. In their approach, a database of high-quality microstructures, represented by ODF, is initially generated using engineering heuristics. The performance of microstructures in the database is evaluated and a random forest model is trained that predicts performances based on samples in the top 10% and bottom 10% performance brackets of the database. Analyzing the trained random forest model allows to automatically generate insights on the most promising exploration directions and re-populate the database with high-performing samples. By repeating with process iteratively, they accumulate high-quality design samples over time. Tamura et al. (2021) implemented a sampling-based method to optimize process parameters in powder manufacturing (gas atomization process) for Ni-Co-based superalloy powder in turbine-disk applications. They used an iterative process where a Bayesian model is trained, potential promising directions are detected, and used to generate new data. Their method resulted in an increased yield of 77.85% from 10%–30% in traditional methods and reduced cost by 72%. More generally, the active learning approach, i.e., using trained models to dynamically adapt and augment the training database, has been explored to complement both surrogate modeling and sampling-based methods, as demonstrated by Lookman et al. (2019) and Tran et al. (2020).

Recent advances in generative models such as variational autoencoders (VAEs) (Kingma and Welling, 2013) and generative adversarial networks (GANs) (Goodfellow et al., 2014) have opened new avenues in manufacturing design. VAEs simultaneously train an encoder and a decoder neural networks to reconstruct the input while the information is passed through a computational bottleneck. GANs, on the other hand, train two competing networks where a generator attempts to produce samples that are indistinguishable from real data while a discriminator learns the discrepancies between the synthesis data from the generator and original data in the database. Both VAEs and GANs produce three valuable assets for engineering design: (1) a latent space that condenses the implicit restrictions and correlations of the design space, (2) a generator/decoder neural network that can map the latent space into the

original design space, and (3) a regressor that can be used in various feature extraction, dimensionality reduction, and classification tasks. While VAEs and GANs offer similar capabilities, VAEs are more known for extracting meaningful and interpretable latent spaces while GANs generally perform better in generating realistic samples.

Generative models can be treated as a source of new designs. To improve the functional performance of generative models, one can iteratively update the database by performance filtering. Shu et al. (2020) developed a self-updating approach where starting from a database consisting of geometrical designs, a GAN model is trained to generate new samples. The new samples are evaluated using a physics-based simulation and the top-performing samples replace parts of the original database. By repeating this process, the design database would be populated with higher quality examples which subsequently leads to a performance-driven GAN model. Oh et al. (2019) optimized for both engineering performance and aesthetics by combining topology optimization and generative modeling in a 2D wheel design case. In their proposed framework, they iteratively apply topology optimization on the GANs output and the original database to create high-quality designs and train GANs to generate samples with high novelty. This process is repeated until a substantial amount of novel and acceptable designs are generated.

Another exciting approach to introduce physical knowledge into generative models is to augment the neural networks and training process with additional terms representing their performance. Chen and Ahmed (2021) developed a GAN model that simultaneously maximizes the diversity, novelty, and performance of generated samples. They augmented the standard GAN loss function with additional terms using determinantal point process (DPP) formulation which encourages the generative network to produce high-quality samples while reducing similarity in a batch of samples. They demonstrate their method for the conceptual design of the airfoil cross-section. Nobari et al. (2021) modified the GAN loss formulation to impose range constraints on 3D geometries and demonstrated their method on producing novel airplanes with an arbitrary range of value and aspect ratio. In Wang et al. (2020), the authors trained a VAE to encode microstructural information into a low-dimensional latent space. They augmented the VAE network that reconstructs a pixelized RVE with a regressor that predicts its stiffness matrix and showed that the latent representation provides a meaningful interpolation of the topological and mechanical properties. As demonstrated in Fig. 16, this method enables producing functionally graded designs in multiscale systems.

5. AI in manufacturing process control and monitoring

5.1. AI in manufacturing process control

Process control is an essential step in manufacturing to ensure the quality and efficiency of a manufacturing process. Due to the strength of AI methods in automatically and efficiently extracting information from big data, AI methods can be applied in manufacturing process control in two primary ways: (1) control-oriented data-driven modeling methods and (2) autonomous decision-making approaches.

A control-oriented model is a model that describes the system behavior and is also suitable in model-based controllers (Landers et al., 2020). As we already discussed previously, physics-based analytical models are often not complete enough to accurately describe manufacturing systems due to their complexity from multiple process variables and uncertainty in the environments. The data-driven methodology can provide an interesting alternative as it can accurately estimate complex states of the dynamical system. Additionally, using data-driven models can be more efficient than solving the full-scale physical-based models, which is an imperative criterion in control tasks.

Several early works have used neural networks to develop data-driven models for manufacturing processes, where the relationship between the input process parameters and output variables is described as a static model, e.g., cutting force (Tandon and El-Mounayri, 2001) and surface finish (Özel et al., 2007) in machining, springback in metal forming (Viswanathan et al., 2003). While these static models provide a basic understanding of the process and could be used for optimizing process parameters (Landers et al., 2020), there are not suitable for designing advanced model-based controllers, e.g., model predictive control (MPC), which requires a dynamic model of the process. The dynamic model of a process can be written as:

$$y_{k+1} = f(y_k, u_k) \quad (4)$$

where y_k and u_k are the output state and control signal at step k . Once the dynamic model is known, the future output state can be predicted. MPC determines the control signal at each time step by optimizing the trajectory over a fixed horizon H :

$$\begin{aligned} \min \quad & L(y_k, u_k, y_{k+1}, u_{k+1}, \dots, y_{k+H}, u_{k+H}) \\ \text{s.t.} \quad & \phi(y_k, u_k, y_{k+1}, u_{k+1}, \dots, y_{k+H}, u_{k+H}) \leq 0 \end{aligned} \quad (5)$$

where L is the cost function and ϕ represent the constraints.

Data-driven models can be applied to identify the dynamics of manufacturing processes for model-based control applications. A stan-

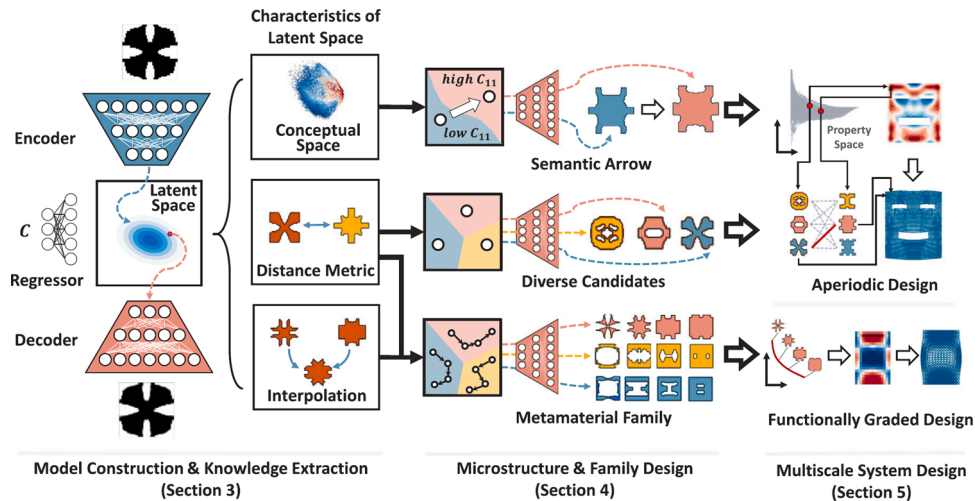


Fig. 16. Variational autoencoder network are trained to identify a dense latent space for microstructure geometry and properties which allows for multiscale microstructure design (Wang et al., 2020).

standard linear model that has been used in manufacturing process control is the auto-regressive model with exogenous inputs (ARX). A general ARX model could be expressed as:

$$y_{k+1} = \sum_{i=1}^{n_a} a_i y_{k+1-i} + \sum_{i=1}^{n_b} b_i u_{k+1-i} \quad (6)$$

where a_i , b_i are the coefficients to be trained. Least-squares regression is usually used to identify the relative coefficients by minimizing the prediction error in the training dataset. An example of this application is presented in (Xia et al., 2020) where they developed a feedback control system to control the melt pool width for the wire arc additive manufacturing process. ARX model is used to model the dynamic relationship between the wire feed speed and the melt pool width and an MPC controller is designed to control the melt pool width.

Using a linear model like ARX can lead to satisfying results if the dynamics in simple and low-dimensional. However, most manufacturing systems are relatively complex with nonlinear effects. Potočník and Grabec (2002) used nonlinear MPC to control the cutting process. A neural network is trained to model the process dynamics and the genetic algorithm is used to solve the nonlinear optimization problem. The NN-based nonlinear MPC is demonstrated in a simulated cutting process to improve the surface quality by preventing tool oscillations.

In the control field, researchers have studied advanced data-driven models such as Gaussian Processes (GPs) (Kocijan et al., 2004), Koopman Operator (Mamakoukas et al., 2020), SINDy (Fasel et al., 2021), and deep neural networks (Lenz et al., 2015) for dynamics system identification. While most of these approaches have been designed in robot control, many of them can be promising methods in manufacturing applications because of the strength in accuracy or training sample efficiency. Lenz et al. (2015) proposed a deep neural network structure for learning the dynamics in the food cutting process. A recurrent structure called Transforming Recurrent Units (TRU) is designed to form the long-term latent features. By incorporating the features from long-term information, short-term dynamic response, and the current control inputs, the dynamic relationship is modeled. A multi-stage pre-training method is proposed where an auto-encoder is used to initialize the non-recurrent parameters in TRU and a then model is pre-trained for single-step prediction before the actual training process. The experimental results show that the proposed model improved the accuracy by 46% compared to the standard recurrent neural network in modeling the dynamic relationships in the food cutting process. Kaiser et al. (2018) proposed SINDy-MPC framework where SINDy is used to identify the dynamics for MPC application. The results show that compared to regular neural networks, SINDy has the strength that it requires a relatively low amount of data. It is also more robust on data with noise and takes lower execution time. Edwards et al. (2021) developed a software package named AutoMPC. ARX, GPs, Koopman Operator, SINDy, and neural network models are implemented in the package and an auto-tuning method is developed. The developed auto-tuning method can help to select the hyperparameters of each model automatically and compare the performance of different system identification models.

The second way that AI can benefit manufacturing process control is to directly learn the control strategy. RL is an emerging tool to perform control. Dornheim et al. (2020) used model-free Q learning to improve the blank holder force optimal control in deep drawing processes. In their proposed approach, the process state is defined as the full information history by concatenating the action history and observable history, where the dimension of the state vector is time-dependent, and a set of neural networks are used to approximate the Q-function at each time step. The RL algorithm is trained and evaluated in the FEM simulation and the results show that, after 200 episodes, it gives better performance than a baseline from an exhaustive search. Ogoke and Farimani (2021) developed an RL framework for melt pool depth control in the laser powder bed fusion process. They deployed Proximal Policy

Optimization (PPO) algorithm to control the scan speed and the laser power in a simulated setting and demonstrated a successful melt pool control with two different toolpath strategies. While both of the above studies executed RL-based control only in simulation, Masinelli et al. (2020) implemented an RL-based feedback control system for welding process in an experimental setting, as shown in Fig. 17. A deep conventional neural network is used to extract the low dimensional features from the monitored acoustic and optic signals, and to classify the signals for forming the rewards by comparing them with a reference signal. Q-learning and Policy Gradient algorithms are tested in experiments and the results show that Q-learning requires less training time and episodes to reach an acceptable performance.

5.2. AI-enabled manufacturing process monitoring

Process monitoring is an important source of information for fault detection, process prognosis, and control in manufacturing systems. Generally, manufacturing process monitoring can be summarized into two levels: (1) observable monitoring (2) unobservable monitoring. The first level is the monitoring of manufacturing process variables that can be directly measured by sensing devices or easily calculated from the sensing signals, such as the cutting force in machining and temperature field in additive manufacturing. The second level includes the monitoring of the process or part conditions that are not directly sensed but could be inferred from the measured information, such as tool condition and defect detection. Traditionally, unobservable monitoring is difficult to achieve because it heavily relies on human interpretation such as image data. In some cases, the features embedded in the data are not even obvious to human experts. With the rapid development of AI and computer vision techniques which have the natural strength to automatically extract features from images, AI-enabled monitoring systems have become widely used in a range of manufacturing processes.

Recently, AI-enabled monitoring have been applied to various manufacturing applications such as tool condition monitoring (e.g., Hesser and Markert, 2019; Li et al., 2019b) and chatter detection (e.g., Tran et al., 2020; Rahimi et al., 2021). Part quality monitoring in additive manufacturing processes is an example of AI-enabled monitoring that has drawn much attention. Scime and Beuth (2018) developed a process image-based defect detection and classification method for powder bed fusion process using an AI algorithm called bag-of-keypoints. The image after preprocessing for eliminating the influence of light conditions is first divided into small patches. 37 different filters are selected and applied to each image patch for feature extraction and the filter response vector of each pixel is are grouped into different clusters using K-means algorithm. A histogram of the percentage of each cluster is created for the image patch and finally, the image patch is classified into categories including anomaly-free, recoater hopping, recoater streaking, debris, super-elevation, part failure, incomplete spreading by comparing the histogram with the database.

Baumgartl et al. (2020) used deep CNN for defect detection in the powder bed fusion process. They used thermal images instead of regular images as the input and trained a model to detect the defect with an accuracy of 96.8%. Scime et al. (2020) developed a pixel-wise semantic segmentation model, called Dynamic Segmentation CNN (DSCNN), for anomaly detection in powder bed fusion process. Their proposed DSCNN model takes different scales of the image and the pixel coordinates as the input to classify each pixel of the image. This is because the pixel is not only influenced by the surrounding pixels but also the global status of the image. A schematic of the proposed architecture is shown in Fig. 18, where four parallel networks are used to extract features at different scales and all the features are concatenated for the final segmentation task.

Supervised learning requires a lot of labeled data for training, and in the monitoring tasks, much of the data needs to be labeled manually. Gobert et al. (2018) used the post-build high-resolution 3D CT data of the AM manufactured parts to generate the ground-truth for the training

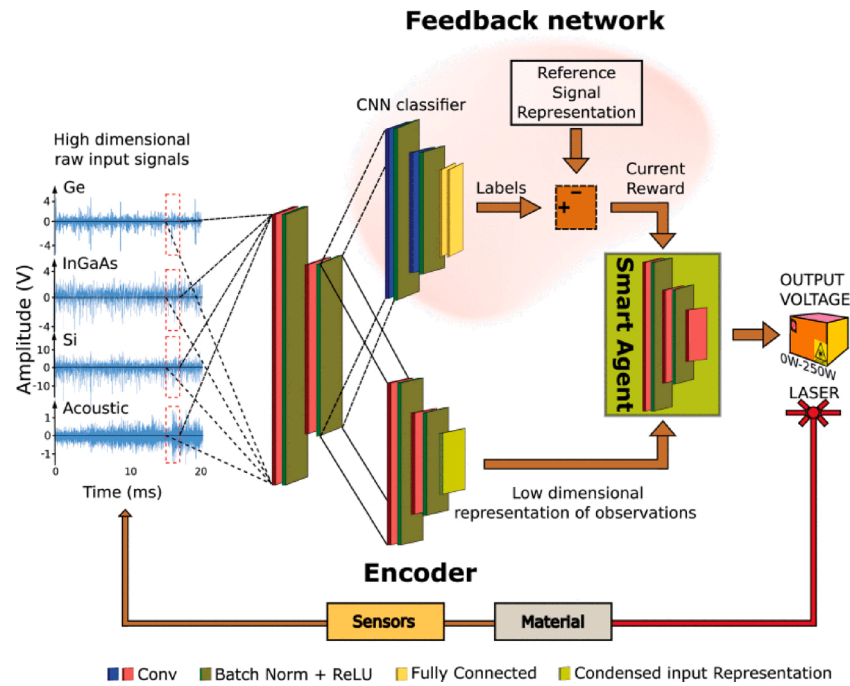


Fig. 17. RL-based feed back control system (Masinelli et al., 2020).

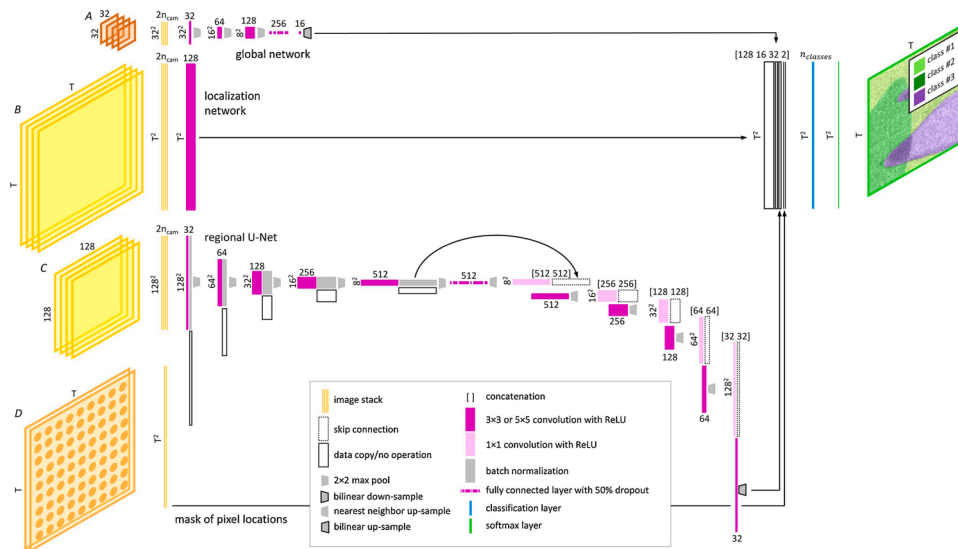


Fig. 18. Structure of Dynamic Segmentation CNN (Scime et al., 2020).

data. The defects are defined as the discontinuity of the scanned voxel data and are automatically calculated and matched with the in-situ images as the label. Westphal and Seitz (2021) used transfer learning to train deep CNN for defect detection. A VGG16/Xception model pre-trained with the ImageNET dataset is used for feature extraction and the final classification layers are only changed for the monitoring task. In the first step of the training, all the pre-trained weights are fixed and only the weights of the classification layers are trained. Later, all weights are set to train simultaneously to fine-tune the model. Furthermore, undersampling and oversampling are used to solve the problem of imbalanced data between normal and defected samples and achieve an accuracy of over 95% while training on 4000 images. Li et al. (2020) proposed an identification consistency-based approach, as shown in Fig. 19 for semi-supervised learning-based defect detection to alleviate the need for large amounts of high-quality labelled data. In this

approach the loss function is designed based on four principles: (1) correct classification of the noisy and blurred image variants from data augmentation (2) consistency of the features extracted from unlabelled image patches and their variants (3) consistency of the features extracted from different patches of the same image (4) diversity of the features extracted from image patches of different images. The result shows that the proposed approach can classify the over-melt, under-melt and well-weld conditions with good accuracy using 1720 image patches from 40 images with labels.

6. Future directions

With the increasing popularity of AI solutions, several research questions arise to address shortcomings of state-of-the-art AI techniques in manufacturing such as lack of interpretability, big data requirements,

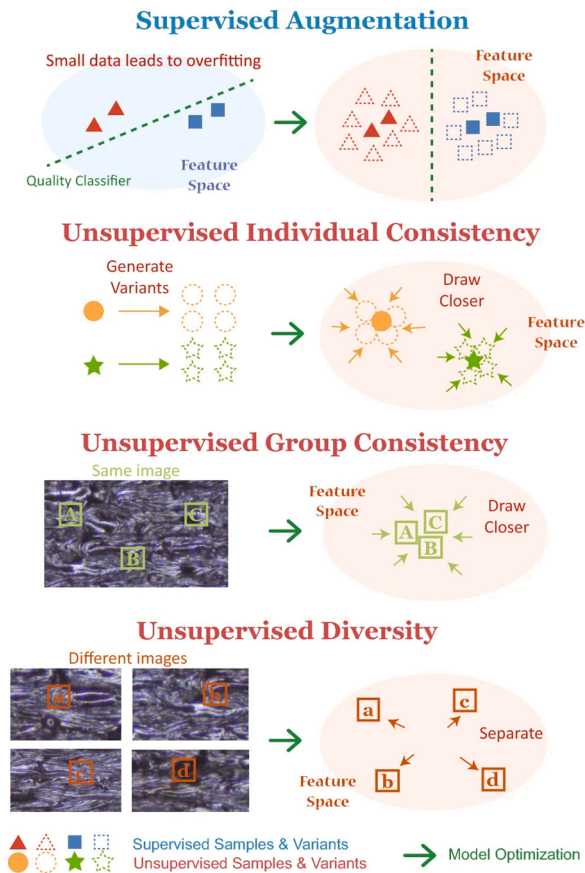


Fig. 19. Overview of the identification consistency-based approach (Li et al., 2020).

limited physical meaning, stability, and generalizability to distributions outside of training data. Our review indicates that Mechanistic-AI approaches are effective steps toward resolving these issues by integrating our knowledge of the data and physics of the process into machine learning solutions. In this section, we summarized the prevailing trends found in this study and discuss promising future research directions.

6.1. Databases, benchmarks, and security in manufacturing data

6.1.1. Need for high-quality experimental and simulation data

Manufacturing involves a wide range of experimental, simulation, and user data. As AI tools are known to be data-hungry, large-scale high-quality and high-resolution measurements and high-fidelity simulations are needed to develop, effectively train, and deploy AI models. Despite the significant progress in the quality and quantity of available manufacturing data, several aspects of the manufacturing data remain challenging. Experimental databases are often unbalanced and prone to human- and sensory-related errors and therefore require massive investment in post-processing and curation (e.g., Freitas and Curry, 2016; Zhang and Gao, 2021). At the same time, simulation data suffer from unknown physics, high computational cost due to the curse of dimensionality, and high variance in their fidelity.

6.1.2. Heterogenous data fusion in deep learning

Some of the challenges stem from the heterogeneous and unstructured nature of manufacturing data where CAD files, simulation data, and various sensory information need to be fused together. If fused properly, these data sources can complement each other's sparsity, accuracy, and uncertainty and create an expanded multi-modal database. While combining data sources in manufacturing has been the topic of several studies (e.g., Lu et al., 2015; Guo et al., 2019) manufacturing

data fusion in the context of AI formulations and methodologies is still an open question. Providing the connections between different data sources so that they hold the spatial and temporal structure of data and avoid information leaks, dilution, and the high noise-to-signal ratio is an understudied topic of research. Additionally, methods to integrate experimental and simulation data are vital in many manufacturing applications not only because collecting experimental data can be prohibitively expensive, but also because the large corpus of available computational methods provides unique insights that are not measurable experimentally.

6.1.3. Reproducibility and established benchmarks

Reproducibility is a major concern in publications addressing AI in manufacturing. Many publications do not share their data, which essentially makes the study unreproducible. Additionally, many AI solutions involve non-trivial implementation details, which significantly affects the final product and how it can be used in practice. The quality of data, the feature processing pipeline, and handling of outlier cases can lead to tangible variations in AI performance. Details of the model (e.g., stateful vs stateless RNN, batch normalization scheme, initialization, model selection to balance precision and recall) and the optimization know-hows (e.g., batching process, gradient clipping, cyclic learning rate) can be the difference between a functional and a nonfunctional AI solution. This problem is particularly pronounced in RL setting where one deals with dynamic data. As these details are often missed from pseudocodes published in papers, we strongly encourage the manufacturing community to publish their implementations and datasets along with their papers. While we observe a surge in the availability of public databases related to manufacturing tasks, they are mostly geared toward geometric analysis and additive manufacturing behavior. Even in those applications, the field lacks established practices for comparing newly proposed methodologies with clear benchmarks. As it stands, most papers in the field are tested on individual databases, which cannot be meaningfully compared to other related works. Although some authors compare their new approaches with their implementation of past methods, a concern can arise that a proposed approach can outperform past work only due to better implementation or more extensive hyperparameter optimization. Having established benchmarks in major manufacturing applications can largely mitigate these concerns.

6.1.4. Biases in manufacturing data

Biases can cause harmful consequences in various stages of the AI life cycle, many of which stem from data collection and curation. Three sources of biases during data preparation are identified in Suresh and Guttag (2019) as representation, measurement, and aggregation biases. Representation bias occurs when the developed database does not sufficiently represent the environment AI solution faces during production. An example of this source of biases is an AI solution that is trained on the data generated by one manufacturing machine (or a small subset of machines) and fails to generalize across larger production facilities. Measurement bias can happen due to not only faulty sensors but also missteps during the preprocessing and feature selection and cause the processed data not to properly estimate the qualities of interest. For instance, various types of measurement techniques with different resolutions and errors might be used to measure the same quantity and introduce a measurement bias in the database. Aggregation bias occurs when data from the larger context is used in a particular application without adjusting the data to capture nuances of the deployment environment. As an example, an AI trained over generic 3D geometries designed for computer vision tasks may extract features focused on visual characteristics of the object and neglect the manufacturability and performance aspects of the analysis. Therefore, a model that is trained, or even pre-trained in a transfer learning fashion, on vision tasks can introduce aggregation biases to manufacturing applications. Therefore, further studies are needed to advance our understanding of the influence

of such biases in critical manufacturing components and effective methods to mitigate them.

6.1.5. Cloud manufacturing and security

Cloud manufacturing is an innovative platform that generates and maintains a large and high-quality database through the cooperation of numerous companies and individuals. Blockchain-based cloud manufacturing is trending recently to decentralize the network and keep security tight. However, even the blockchain technique cannot prevent a data breach (i.e., unauthorized access to the database, retrieval, or modification of the data) that happens inside a company by malicious insiders such as past employers and business competitors. The data breach might cause a serious data loss or falsification, leading to a tremendous economic loss. To prevent and prepare for the data breaches, (Esposito et al., 2016) proposed two crucial steps. Firstly, a proper key management system should be developed inside a company. The system records who have the key and revokes the keys if not used. Secondly, companies should be able to detect a data breach, notify related personnel, and record them forensically to prepare for a lawsuit. As a little volume of studies has been reported in the area of data breach prevention in manufacturing, further studies should be conducted in this area.

6.2. Data-driven modeling and discovery in manufacturing

6.2.1. Frameworks for mechanistic feature selection

Extraction of mechanistic features still relies on domain experiences. Selecting appropriate mechanistic features for complex problems could be very challenging. Developing systematic data-driven approaches, which can automatically identify dominant mechanistic features from different manufacturing data sources, is an interesting topic. Moreover, the extracted mechanistic features might have various physical dimensions (or units). Dimensional analysis (Barenblatt, 2003) can be a very useful principle to guarantee the dimensional homogeneity (Rudolph et al., 1996) of the discovered relationships.

6.2.2. Large-scale Mechanistic-AI modeling in manufacturing

Mechanistic-AI methods have the potential to capture complex process-structure-properties relationships in advanced manufacturing. They can tackle the problems with missing/noisy boundary conditions and material laws, which are currently impossible or extremely expensive to solve through traditional methods. However, embedding physical, chemical, and material mechanisms into AI systems remains a non-trivial task. Researchers have proposed several approaches, such as mechanistic feature extraction, specialized network architecture, and regularization of loss functions. Much effort needs to be directed at improving the developed methods to solve real manufacturing problems with high uncertainty and variability during the processes.

6.2.3. Extension of PINNs to manufacturing applications

Physics-informed neural network has been successfully applied to additive manufacturing. It can be extended to broader manufacturing techniques, such as metal forming, welding, and micro-manufacturing. A challenge is to improve the generalization capabilities of PINN (Raissi et al., 2019), especially for the problems with complex geometry and transient boundary condition.

6.2.4. Advance transfer learning using highly generalizable models

Transfer learning is another interesting future direction. Transferring trained models and identified knowledge from one material to another or from one manufacturing technique to another is currently extremely challenging. Dimensionless scale-invariant relationships play an important role in properly transferring knowledge because they offer better generalization capability compared to transitional empirical equations.

6.2.5. Data-driven physics discovery

Data-driven discovery, such as SINDy method (Brunton et al., 2016), is a very promising approach to discover new underlying physical, chemical, and material mechanisms from noisy manufacturing data. Generating more high-quality in-situ experimental data and high-fidelity simulation data is crucial in the near future. Data-driven dimensional analysis is another important area that requires significant improvements in the future. The developed algorithms can be used to discover more universal dimensionless numbers and scaling laws from manufacturing processing data, which provides a smaller set of parameters to describe the highly multivariable manufacturing processes. It is noted that describing or predicting the widest range of phenomena with a minimum of variables is always the central goal in science and physics (Kunes, 2012).

6.3. Data-driven design methods in manufacturing

6.3.1. Supervised learning and constraint satisfaction for design

Design in manufacturing is challenging due to the high-dimensional spaces and discreet choices involved as well as the complexity of the physical mechanisms during the manufacturing processes. Mechanistic-AI methods have the potential to efficiently solve inverse problems with hidden physics for process design. Several papers have explored the potential of AI methods to solve manufacturing design problems by (1) establishing a direct mapping between functional requirements and design parameters, or (2) formulate an optimization problem to explore the design space. Supervised learning has shown to be an effective tool to extract correlational requirement-to-design parameter relationships. However, state-of-the-art practices lack incorporating physical constraints of the problem into the learning method. As the result, these methods are only reliable for problems with simple constraints or within a limited range of parameters. As an example, consider the problem of toolpath design to achieve favorable material behavior. We can generate a database of tool paths and their resulting material properties and train a model to produce a toolpath given the properties. Naturally, the supervised learning method interpolates between database points, which can easily lead to physically unfeasible or overlapping tool paths. Therefore, studying representations in which such interpolation is valid or approaches to enforce physical constraints is a crucial step in broadening the applications of supervised learning in design. Various ideas in physics-informed modeling techniques (as reviewed in Section 3.2) can be deployed in design applications to soft or hard impose the constraints.

6.3.2. Reinforcement learning in design

RL offers an alternative to supervised learning when the design involves a sequential decision-making process. Constraints can be implicitly introduced into the solution by penalizing constraint violations. However, RL methods are known for their poor sample efficiency. Furthermore, as RL methods explore many unfeasible and potentially dangerous design spaces, they can rarely be trained on experimental manufacturing setups. To address these challenges, future research is needed to expand the capabilities of off-policy RL methods to allow training on historic data and enable data reuse. Additionally, further investigations need to bridge the gap between RL methods trained on simulation environments and real setups. While several examples of RL in manufacturing were presented in Section 4.1, the performance of RL agents heavily depends on the quality of reward function to break down the complexity of the overarching goal. As many manufacturing decision-making processes involve sparse signals where the goals cannot be trivially divided into subtasks, advancements in sparse credit assignment are vital in the future. Model-based RL has the potential to address some of these challenges. As an alternative to purely explorative methods, model-based RL can utilize its underlying model to perform look-ahead planning and search (e.g., Monte Carlo Tree Search) and therefore offer better sample efficiency and compatibility with reward

sparsity.

6.3.3. Process-informed design exploration using generative models

Recent advancements in generative models, such as GANs, opened new possibilities to discover condensed latent design spaces. While recent studies have expanded the capability of GANs and VAEs to generate high-quality designs by incorporating performance metrics, much of the focus has been dedicated to esthetic and geometric features. The extension of generative methods to complex physical aspects of manufacturing processes has remained unsolved. Therefore, a promising future direction is physics-informed generative models that leverage PINN in GANs training to facilitate extracting generalizable and physically valid correlations.

6.3.4. Uncertainty quantification in scientific deep learning

Despite tremendous progress in manufacturing process modeling and design using AI, most of these studies lack uncertainty analysis or quantification in their deep learning framework. However, in manufacturing, it is often critical and expected to assess the reliability of deep learning models before they are deployed (Jiang et al., 2018). Uncertainty analysis in deep learning methods has attracted several research ideas in computer vision (Michelmoro et al., 2018), medical image analysis (Kwon et al., 2020), and natural language processing (Xiao and Wang, 2019) with Bayesian approximation (Gal and Ghahramani, 2016) and ensemble learning techniques (Lakshminarayanan et al., 2016) as the two most widely used uncertainty quantification methods. Several state-of-the-art trends in deep learning uncertainty quantification are reviewed by Abdar et al. (2021). Therefore, we believe rigorous uncertainty analysis in the context of AI solutions in manufacturing is a vital topic for future research which can significantly accelerate the industrial adoption of the field.

6.3.5. Lack of integrated design steps

Many methods have been emerged to provide an integrated design than an individual design task (e.g., conceptual design, process planning, process parameter optimization). However, we find insufficient research effort into integrating multiple design steps. The interconnectivity of manufacturing design tasks is a key reason behind its complexity. AI methods have caused a fundamental shift from solutions with numerous subtasks to overarching end-to-end systems. We believe future research into end-to-end design methods that bridge between intertwined manufacturing design tasks can be profoundly influential in the field.

6.4. Data-driven control and monitoring in manufacturing

6.4.1. Adoption of advanced Mechanistic-AI in control

It is commonly acknowledged that process control is a crucial component in manufacturing processes that can improve the quality and stability of a manufacturing process. AI techniques have been and will be increasingly applied to manufacturing process control because of their ability to handle and learn information from big data. Most of the current literature on model-based manufacturing process control utilizes linear models or relatively simple data-driven models, such as ARX model, for modeling the system dynamics. It has been shown that AI techniques such as SINDy and deep neural networks can be effectively used to model system dynamics and have been applied in the control of robots and autonomous vehicles. We expect future research in manufacturing process control will adopt these techniques to control-oriented manufacturing modeling to achieving better accuracy and efficiency. Additionally, as the current literature solely deploys physics-based or data-driven models, we believe hybrid Mechanistic-AI models can advance current control capabilities in the field.

6.4.2. Efficient reinforcement learning for control

While RL methods can be used in manufacturing process control

without knowing the system model, there is currently limited application in the real manufacturing process because of the high cost to train the model. Previous research has implemented RL-based process control on top of simulations with hundreds of episodes and it will be extremely expensive in the real world. How to train an RL model with good accuracy using combined a large amount of simulation data and a relatively small amount of experimental data will be an important field to explore.

6.4.3. Auto-labeling and efficient learning in process monitoring

For the process monitoring, a lot of current work used supervised learning to train a model that can identify the process condition from images, where a large number of labeled images are required for training. Thus, questions such as how to efficiently get enough labeled data for training, and how to train a model with less labeled data, need to be further studied.

6.4.4. Robustness in AI process monitoring

In most studies on AI-enabled process monitoring, the model is trained and tested on the prepared dataset, and has not been validated and applied to experimental or industrial setups. One reason for this gap between research and industry is that oftentimes the trained model is sensitive to the environmental condition. Therefore, when the environmental condition is changed or a different machine is used for the same process, the model is no longer accurate. In the past few years, methods like stability learning (Zheng et al., 2016) and Parseval networks (Cisse et al., 2017) attempted to address these challenges with limited success. We believe that improving the robustness of the AI-enabled process monitoring techniques to make them more applicable in real industry settings will be an important future direction.

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Conflict of interest

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

Declaration of Competing Interest

The authors report no declarations of interest.

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