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An optimization-centric review on integrating artificial intelligence and digital twin technologies in manufacturing

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ABSTRACT

This article reviews optimization methods that enhance adaptability, efficiency and decision making in modern manufacturing, emphasizing the transformative role of artificial intelligence (AI) and digital twin technologies. By integrating AI and machine learning algorithms within digital twin frameworks, manufacturers can facilitate real-time monitoring, quality control and dynamic process adjustments. This synergy not only boosts operational efficiency but also enables precise modelling, offering predictive insights for strategic planning and innovation. The combination of digital twins and optimization techniques supports resource optimization, balancing competing objectives and driving continuous process improvements. With both offline and online optimization approaches, digital twins enable efficient production adjustments while ensuring long-term performance and scalability. Ultimately, this review highlights digital twins as foundational technologies for smart, sustainable manufacturing, incorporating advanced optimization strategies to enhance adaptability and operational resilience. This positions optimization algorithms and digital twins as key drivers in the future of intelligent production systems.

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Digital twins; optimization; artificial intelligence; manufacturing systems and machine learning

1. Introduction

The manufacturing landscape is currently undergoing a significant transformation, propelled by the integration of digital technologies that enable sophisticated real-time monitoring, in-depth data analysis and continuous process optimization (Jiao *et al.* 2021). At the forefront of this revolution are artificial intelligence (AI), machine learning (ML) and digital twin technologies, each playing a pivotal role in building manufacturing systems that are not only efficient but also agile and scalable. These advances have moved from being technological enhancements to essential components in an increasingly competitive global market. Digital twins, in particular, have emerged as a cornerstone in the vision of smart manufacturing, serving as virtual replicas of physical assets that provide predictive insights, optimize operational workflows, and facilitate rapid adaptation to fluctuating conditions and requirements (Behie *et al.* 2023).

According to the National Academy of Sciences report on Digital Twins, a digital twin is defined as a dynamic, virtual representation of a physical system (Adhikari 2021; National Academies of Sciences, Engineering, and Medicine, 2024). This virtual construct integrates real-time data from sensors and historical information to closely mirror the physical system's behaviour, context and structure. Digital twins go beyond traditional simulations by enabling bidirectional data exchange, meaning that they continuously update based on real-world changes and can inform physical systems

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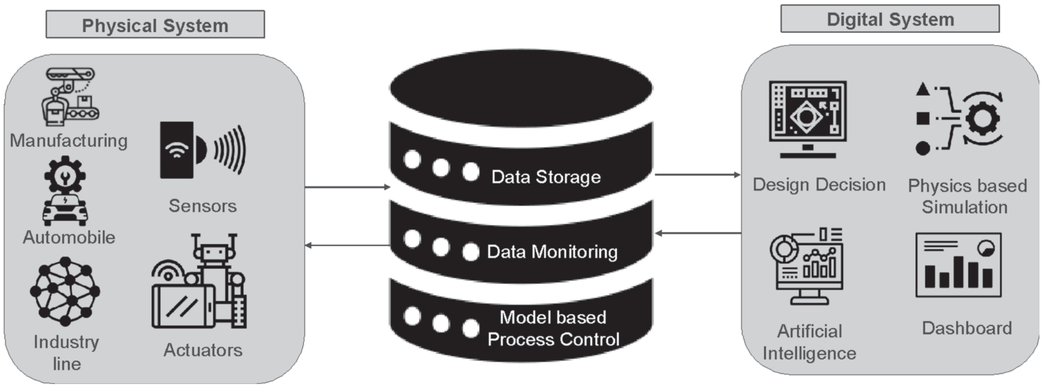

Figure 1. Outline of a digital twin framework, showing the interaction between physical manufacturing elements and digital systems, enhancing operational efficiency through real-time data analysis and decision making.

through predictive insights, optimizing performance and allowing for proactive adjustments in various applications (Adhikari 2021; National Academies of Sciences, Engineering, and Medicine, 2024). This digital representation allows manufacturers to simulate, analyse and optimize systems with unparallelled precision, transforming traditional reactive maintenance approaches into predictive and prescriptive strategies. As manufacturing continues to evolve, the role of optimization within digital twin frameworks becomes increasingly critical for streamlining production design, boosting operational efficiency and enhancing long-term strategic planning (van Beek, Nevile Karkaria, and Chen 2023). Optimization methods empower digital twins to act as decision-support tools, enabling manufacturers to improve resource utilization, anticipate potential issues and enhance overall production outcomes.

Figure 1 illustrates a digital twin framework, demonstrating the interaction between physical and digital systems. The physical side includes manufacturing elements such as sensors and actuators, which feed data into the digital side, where they are stored and analysed (Javaid *et al.* 2021). Key digital components include model-based process control, AI and physics-based simulations, supported by comprehensive dashboards for real-time decision making and monitoring (Mihai *et al.* 2022). This integration enhances operational efficiency by mirroring physical processes in a digital environment but also enabling rapid updates and continuous twinning, ensuring that the digital twin accurately reflects real-time changes in the physical system (He and Bai 2021).

The ability of digital twins to perform real-time optimization is a big advantage in manufacturing. By continuously employing AI and ML algorithms, these digital systems can adjust operational parameters instantaneously, based on live data inputs. Optimization algorithms allow digital twins to adapt to both micro- and macro-level changes within the manufacturing environment, enabling dynamic process improvements and minimizing disruptions. This adaptability is crucial in modern manufacturing, where flexibility and responsiveness are key to maintaining a competitive edge. Furthermore, by balancing competing objectives, such as cost, quality and production speed, optimization techniques integrated into digital twins facilitate a more holistic approach to process management and decision making.

The application of AI and ML in manufacturing is transforming traditional methods, driving the shift towards more agile and adaptable manufacturing systems (ElMaraghy *et al.* 2021). Moreover, the application of optimization techniques in digital twins extends beyond immediate process enhancements, encompassing a broad range of strategic objectives, including sustainability, energy efficiency and risk mitigation (Kang, Catal, and Tekinerdogan 2020). Furthermore, the integration of ML techniques with robotics has led to the development of autonomous robots that can perform complex assembly tasks with precision and flexibility (Alexopoulos, Nikolakis, and Chryssolouris 2020). Digital twin technology complements these innovations by creating virtual replicas of physical systems, allowing manufacturers to test and modify processes in a simulated environment before actual implementation (Z. Huang *et al.* 2022). This integration significantly enhances operational efficiency and reduces time to market, providing a robust framework for continuous improvement and innovation. In addition, a digital twin framework for model predictive control (MPC) of process parameters aims to optimize performance and material properties by integrating real-time monitoring with ML models (V. Karkaria, Goeckner, *et al.* 2024).

Previous review articles (Botín-Sanabria *et al.* 2022; Cimino, Negri, and Fumagalli 2019; M. Liu *et al.* 2021; Rathore *et al.* 2021; VanDerHorn and Mahadevan 2021) have highlighted the growing importance of digital twin technologies in the context of Industry 4.0, with a particular focus on modelling, simulation and optimization across various industries. These studies underscore the transformative potential of AI, ML and digital twins in reshaping global manufacturing practices. Advanced optimization methods, such as multi-objective algorithms, genetic algorithms and MPC, enable digital twins to tackle complex trade-offs between operational goals. This capability ensures that manufacturing systems not only meet current performance standards but also align with long-term environmental and economic goals. In particular, multidisciplinary optimization methods allow for the seamless integration of diverse manufacturing aspects, such as thermal dynamics, structural integrity and material properties, making digital twins powerful tools for holistic manufacturing optimization.

This article explores the critical role of optimization methods within digital twin frameworks and their transformative potential for the manufacturing industry. By examining various optimization techniques and their integration with AI and ML models, this research seeks to highlight how digital twins can maximize manufacturing efficiency and performance. This exploration addresses key challenges, such as managing system complexity, handling data variability and improving predictive accuracy. Through a detailed analysis, this article provides insights into how optimization, AI and digital twin technologies can be effectively combined to achieve sustainable and intelligent manufacturing systems. By delving into the synergistic relationships between these technologies, the importance of a cohesive, optimized digital twin framework for the future of manufacturing is underscored. The critical questions posed in this article are as follows.

(A) How can AI and advanced ML techniques be optimized to efficiently process real-time data, enhance predictive accuracy, and maintain effective decision-making and optimization capabilities within digital twin frameworks for manufacturing?
This question explores the development of AI-driven digital twins that not only simulate and control manufacturing processes but also handle large-scale, complex, real-time data streams with efficiency. It investigates how AI and sophisticated ML models can dynamically interpret diverse data sources, optimize production outcomes and predict system failures with greater accuracy. It also focuses on enabling these models to make informed, real-time decisions, ensuring that digital twins remain effective in ongoing optimization and responsive to the evolving needs of manufacturing operations (Uhlemann *et al.* 2017; van Beek, Nevile Karkaria, and Chen 2023). The solutions and approaches to this question will be discussed in Section 4.1.

(B) How can foundation models be adapted and optimized within digital twin frameworks to enhance scalability, generalization and decision-making capabilities across diverse manufacturing scenarios?
This question examines the potential for using large, pretrained foundation models as integral components of digital twins, focusing on decision making and optimization. It explores how these models can be adapted and optimized for various manufacturing contexts, allowing digital twins to scale effectively and generalize across different environments. This minimizes the need for extensive retraining and maximizes operational efficiency, enabling digital twins to provide robust decision-making support and dynamic optimization across a wide range of manufacturing scenarios (Bommasani *et al.* 2022). The solutions and approaches to this question will be discussed in Section 4.2.

(C) How can a networked system of digital twins be optimized to collaborate effectively, sharing insights and enhancing processes across multiple manufacturing sites, while maintaining effectiveness in decision making and optimization?
This question explores the orchestration of interconnected digital twins, emphasizing the optimization of communication protocols, algorithms and data-sharing techniques. The goal is to enable these systems to work together seamlessly, optimizing workflows and enhancing decision making and overall manufacturing efficiency on a large scale. By facilitating real-time collaboration, these networked digital twins can ensure continuous optimization and provide robust support for decision making across diverse manufacturing scenarios (Ramu *et al.* 2022). The solutions and approaches to this question will be discussed in Section 4.3.

(D) How can uncertainty in predictive modelling be quantified and managed within digital twin systems to ensure reliable and optimized manufacturing outcomes, while maintaining effectiveness in decision making and optimization?
This question focuses on identifying and developing methods to accurately measure and incorporate both epistemic and aleatoric uncertainties into the simulations and predictions made by digital twins. It also explores how managing these uncertainties can improve the robustness and trustworthiness of the insights provided by digital twins, enabling them to maintain effective decision making and continuous optimization within manufacturing environments (Thelen *et al.* 2023). The solutions and approaches to this question will be discussed in Section 4.4.

(E) How can offline optimization techniques be effectively used within digital twin frameworks to enhance system performance, validate control strategies and ensure robust predictive capabilities in manufacturing settings?
This question investigates the role of offline optimization in the context of digital twins, focusing on techniques that use historical data and computationally intensive methods to optimize various aspects of manufacturing. It examines how these techniques can refine control parameters, improve model accuracy and support decision-making processes. By doing so, offline optimization enables digital twins to deliver optimized strategies that can be applied in real-world systems, maximizing efficiency and ensuring that digital twins provide reliable, actionable insights to support manufacturing operations. The answer to this question will be discussed in Section 5.

(F) How can real-time process control be integrated with digital twins to optimize manufacturing performance?
This question investigates the application of real-time process control (*e.g.* MPC) within digital twins, focusing on how this integration can be optimized to fine-tune operational parameters and material properties, thereby improving product quality and reducing time to market (McClellan *et al.* 2022). The solutions and approaches to this question will be discussed in Section 6.

(G) What are the most effective design strategies for co-designing the materials and processes to optimize material properties?
The traditional approach is to design materials and process conditions, followed by real-time control for the processes, leading to suboptimal solutions. This question highlights the importance of integrating decision-making problems across different stages and how this integration can improve the ultimate outcome using control co-design (CCD) frameworks. Owing to the distinct natures of design problems (*e.g.* online *vs* offline decision making, time-dependent *vs* time-independent variables), developing a generalizable framework remains a significant challenge (Garcia-Sanz 2019). A detailed discussion of the solutions and methods related to this question can be found in Section 6.3.

This article covers several key areas that are critical to the optimization of digital twin technologies within modern manufacturing environments. First, it explores the role of AI, ML and optimization techniques in enhancing digital twin frameworks by focusing on real-time data processing, predictive accuracy and dynamic control of manufacturing processes. The article also delves into foundation models, examining their scalability and adaptation across various manufacturing contexts, and how these models can be optimized for efficiency and performance. Furthermore, this research investigates the networking of multiple digital twins and how collaboration across manufacturing sites can improve system-wide performance. In addition, the challenges of uncertainty quantification, MPC and the integration of real-time optimization methods are discussed to ensure reliable and optimized outcomes. Ultimately, the article aims to provide a comprehensive understanding of the strategic role that digital twins play in modern manufacturing systems, while also identifying the future research directions required to maximize their potential. Each of these questions seeks to push the boundaries of current manufacturing technologies and provide a roadmap for future innovations in the field. By addressing these gaps, this research aims to advance the scientific and technological foundations necessary for the next-generation digital twin capabilities that will define the future of manufacturing.

2. Roles of optimization methods for digital twins in manufacturing

Optimization methods play a crucial role in enhancing the capabilities of digital twins in manufacturing. They ensure that manufacturing systems can adapt to real-time changes, improve decision making and achieve long-term efficiency. These methods help in refining processes, managing uncertainties and optimizing various aspects of the manufacturing environment. The key roles of optimization methods within digital twin frameworks in manufacturing are listed as follows.

(1) Facilitating real-time process optimization: Optimization methods enable digital twins to make immediate adjustments to manufacturing processes by utilizing real-time data from sensors and other inputs. This role is essential in maintaining operational stability, minimizing disruptions and dynamically optimizing production, ensuring that systems respond quickly to any changes in the manufacturing environment (Davis *et al.* 2012).
(2) Providing flexibility and scalability: The role of optimization methods is to ensure that digital twins can scale and adapt to varying production requirements and system complexities. Whether handling different production scales, materials or operational constraints, these methods allow digital twins to remain flexible and relevant, enhancing their ability to optimize both small- and large-scale manufacturing operations (Putnik *et al.* 2013).
(3) Enhancing predictive accuracy through AI integration: Optimization methods enhance the predictive accuracy of digital twins by integrating with AI and ML models. These models continuously improve their predictions through optimization, providing better control in real-time operations and informing more effective long-term planning and decision-making processes (Leng *et al.* 2021).
(4) Managing uncertainty and risk in manufacturing: A critical role of optimization methods is to help digital twins to manage the inherent uncertainties in manufacturing processes. These methods allow digital twins to quickly adapt to real-time variability and mitigate risks, while also enabling comprehensive scenario analysis for future uncertainties, ensuring robustness in both operational and strategic contexts (Mahadevan, Nath, and Hu 2022).
(5) Balancing multiple objectives in manufacturing: In complex manufacturing systems, there are often competing objectives, such as cost reduction, quality improvement and production speed. Optimization methods enable digital twins to balance these objectives effectively, providing solutions that address both immediate operational needs and long-term strategic goals (Tronsen 2023).
(6) Supporting multidisciplinary optimization: Optimization methods allow digital twins to integrate multiple disciplines, such as mechanics, thermal dynamics and control systems, to manage complex processes in manufacturing. By optimizing these interdisciplinary factors, digital twins can enhance overall system performance and ensure better outcomes in advanced manufacturing environments such as additive manufacturing (Y. Wu *et al.* 2022).
(7) Driving continuous improvement through learning: Optimization methods play a role in fostering continuous learning and improvement for digital twins. By analysing real-time and historical

data, optimization techniques help digital twins to evolve over time, leading to improved processes and better decision making in future operations (Lin *et al.* 2021).

(8) Ensuring efficient resource utilization: One of the key roles of optimization methods is to ensure the efficient use of resources such as energy, materials and time. In real-time applications, these methods enable quick decision making that maximizes resource utilization, while offline optimization refines strategies for more efficient future operations (Goodwin *et al.* 2022).

(9) Facilitating integration across manufacturing systems: Optimization methods must ensure seamless integration with existing systems such as manufacturing execution systems, enterprise resource planning and supply-chain management (SCM) tools. This role is crucial in enabling digital twins to enhance system-wide performance improvements, both in real time and during long-term strategic planning (K. Zhang *et al.* 2020).

In conclusion, optimization methods are essential for enabling digital twins to operate efficiently and adaptively in real time while driving long-term improvements in manufacturing systems. By addressing the complexities and challenges of modern manufacturing, these methods enhance productivity, reduce risks and improve overall operational performance.

3. Challenges for effective optimization in digital twins

Integrating optimization techniques within digital twin frameworks offers substantial potential for improved efficiency, responsiveness and decision making in manufacturing. However, realizing these benefits involves overcoming several significant challenges:

(1) Data quality and consistency: Effective optimization relies heavily on high-quality, consistent data from multiple sources, such as Internet of Things (IoT) devices and historical databases (Younan *et al.* 2020). Variations in data formats, quality and frequency across different stages of manufacturing can obstruct the optimization process (Kumar *et al.* 2023). Ensuring that data are cleaned, standardized and reliable is critical yet challenging, especially in real-time environments (Karkouch *et al.* 2016).

(2) Complexity of multi-scale modelling: Digital twins often need to simulate processes at different scales, from microscopic material properties to large-scale production systems (Castelló-Pedrero, García-Gascón, and García-Manrique 2024; Gunasegaram *et al.* 2021). Optimization across these scales requires diverse techniques that can balance computational resources and ensure accuracy (Villalonga *et al.* 2021). This adds complexity, as cohesive models must handle both broad and detailed simulations efficiently (Lei *et al.* 2023).

(3) Adapting to rapid technological changes: Manufacturing continuously evolves with the introduction of new technologies, materials and processes (Grodal, Krabbe, and Chang-Zunino 2023; Kanishka and Acherjee 2023). Digital twins need flexible and adaptive algorithms to keep pace with these advances (L. Liu *et al.* 2022). Ensuring that optimization techniques remain relevant as new methods emerge requires frequent updates and adjustments (Javaid, Haleem, and Suman 2023).

(4) Resource and energy optimization: With a growing focus on sustainability, digital twins are increasingly used to optimize both resource use and energy consumption (Bortolini *et al.* 2022; V. Karkaria *et al.* 2023; Teng *et al.* 2021). Balancing high performance with environmental efficiency often involves trade-offs between operational speed and energy usage (Bo and Yi 2024; Godse *et al.* 2021). Advanced multi-objective optimization techniques are essential for navigating these competing demands, adding complexity to the process (C. Wu *et al.* 2021).

(5) Handling nonlinearities and interdependencies: Manufacturing processes often include complex, nonlinear relationships between components (Thelen *et al.* 2022). Optimization algorithms need to account for these interdependencies, requiring advanced methods capable of

capturing nonlinear dynamics and making real-time adjustments (Maier *et al.* 2014). This necessitates sophisticated approaches, such as genetic algorithms and neural networks, which can be computationally demanding (Wen, Gabrys, and Musial 2022).

(6) Predictive maintenance and downtime minimization: Digital twins are commonly used to predict maintenance needs and minimize downtime (Errandonea, Beltrán, and Arrizabalaga 2020; V. Karkaria, Chen, *et al.* 2024; Z. Liu, Meyendorf, and Mrad 2018; van Dinter, Tekinerdogan, and Catal 2022). Optimizing models to align maintenance with production schedules is challenging, as it requires integrating ML algorithms that analyse real-time equipment data and synchronize maintenance activities to minimize disruptions (Negri *et al.* 2021).

(7) Integration with legacy systems: Many manufacturing facilities operate with legacy systems that are not readily compatible with modern digital twin technologies (Lattanzi *et al.* 2021). Ensuring optimization across these systems requires interoperability solutions, such as middleware and data standardization tools, which allow digital twins to connect seamlessly with older equipment and software (Semeraro *et al.* 2021).

(8) Cybersecurity and data privacy in optimization models: As digital twins increasingly rely on cloud computing and real-time data sharing, cybersecurity and data privacy become essential concerns (Alcaraz and Lopez 2022; de Azambuja *et al.* 2024; Lampropoulos and Siakas 2023; Y. Wang *et al.* 2023). Protecting sensitive manufacturing data while allowing optimization models to process and share them requires robust security protocols, including encryption and secure application programming interfaces (APIs), as well as compliance with data protection standards (Domingo-Ferrer *et al.* 2019).

To address these challenges, this article presents three categories of solutions: modelling, offline optimization and online decision making, which are organized in Figure 2. First of all, modelling approaches are investigated to build accurate and adaptive representations of the system. Several optimization algorithms are discussed for offline optimization and can be used to identify optimal configurations and enhance performance. Complementing these efforts, online decision-making strategies, including adaptive learning, real-time process control and co-design of materials and processes, enable dynamic adjustments during operation, helping to achieve adaptable digital twin systems.

4. Solutions for modelling approaches of digital twins frameworks in manufacturing

To ensure that future manufacturing systems are optimized for real-time efficiency and adaptability, users must integrate advanced digital twin technologies with AI and ML, focusing on improving predictive accuracy and decision-making capabilities. These digital twins act as dynamic, real-time virtual models of physical systems, using vast data streams to optimize operations, reduce uncertainties and enhance system performance. By utilizing scalable data architectures, edge computing and continuous learning mechanisms, manufacturers can implement actionable strategies for predictive maintenance, system optimization and rapid response to evolving operational challenges. This approach strengthens the adaptability and robustness of manufacturing processes, ensuring sustainable and innovative production models.

4.1. Improving digital twins with fast machine learning models for manufacturing state tracking and prediction

In the rapidly evolving landscape of advanced manufacturing, especially in domains such as additive manufacturing (AM), the need for fast ML models is becoming increasingly critical for optimizing digital twin systems. For instance, in AM, where the precision of layer deposition and thermal management directly impacts product quality, real-time data tracking and prediction are essential. Improving predictive systems through AI involves developing custom AI models specifically tailored

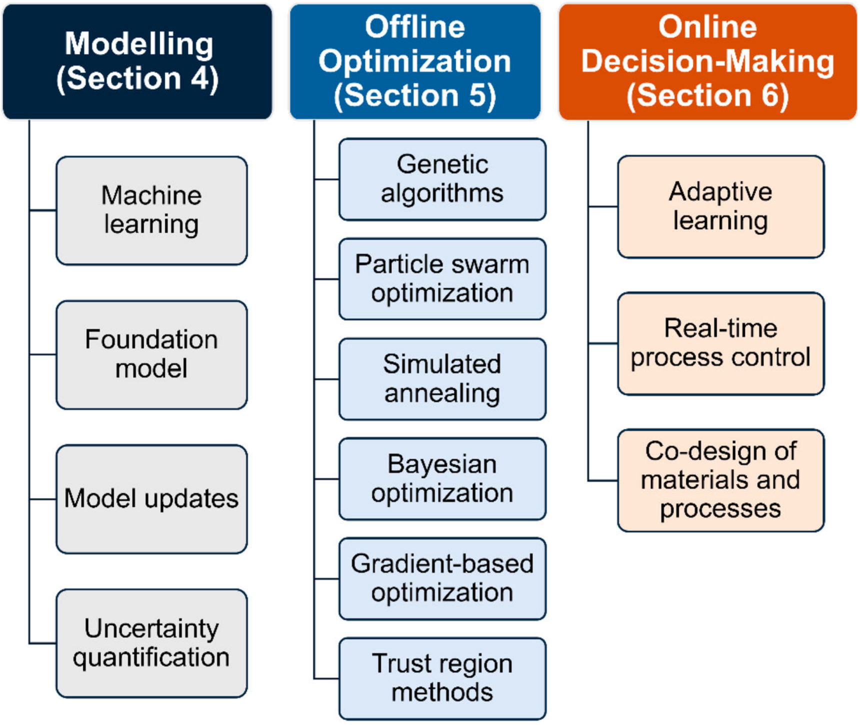

Figure 2. Summary of solutions for realizing digital twin frameworks in manufacturing.

for digital twin applications to enhance predictive accuracy concerning system failures, maintenance needs and process optimization (van Dinter, Tekinerdogan, and Catal 2022). These models are crucial as they use both historical and real-time operational data to forecast potential disruptions, thereby enabling pre-emptive adjustments that can prevent costly downtimes and prolong equipment lifespan (Zacharaki *et al.* 2021). By integrating advanced ML algorithms, such as recurrent neural networks (RNNs), long–short-term memory (LSTM) networks and transformers, which are particularly effective for time-series data, digital twins can continuously learn and adapt to new patterns, improving their predictive accuracy over time (Essien and Giannetti 2020; Reimer *et al.* 2022). Recent advances in LSTM architectures, such as the extended long–short-term memory (xLSTM), have introduced modifications such as exponential gating and novel memory structures, enhancing the model's ability to capture complex temporal dependencies (Alharthi and Mahmood 2024). In addition, the temporal fusion transformer (TFT) combines high-performance multi-horizon forecasting with interpretable insights into temporal dynamics, making it particularly effective for time-sensitive manufacturing tasks and predictive analytics within digital twins (V. Karkaria, Goeckner, *et al.* 2024; Lim *et al.* 2021).

The importance of employing fast surrogate models in this context cannot be overstated. Surrogate models, such as Gaussian processes (GPs) or simplified neural networks, are used to approximate the behaviour of complex systems quickly and with reduced computational costs (Chakraborty and Adhikari 2021). These models are essential for scenarios where real-time decision making is critical, as they allow for rapid predictions that can be crucial for operational management and immediate response strategies. Furthermore, regular model updates are necessary to maintain the accuracy and relevance of the predictive models (J. Q. Wang, Du, and Wang 2020). Techniques such as online learning, where the model is continuously updated as new data come in, and transfer learning, which adapts pretrained models to new but related tasks, are vital for keeping the digital twin models effective as the operational environment evolves (H. Zhang *et al.* 2023).

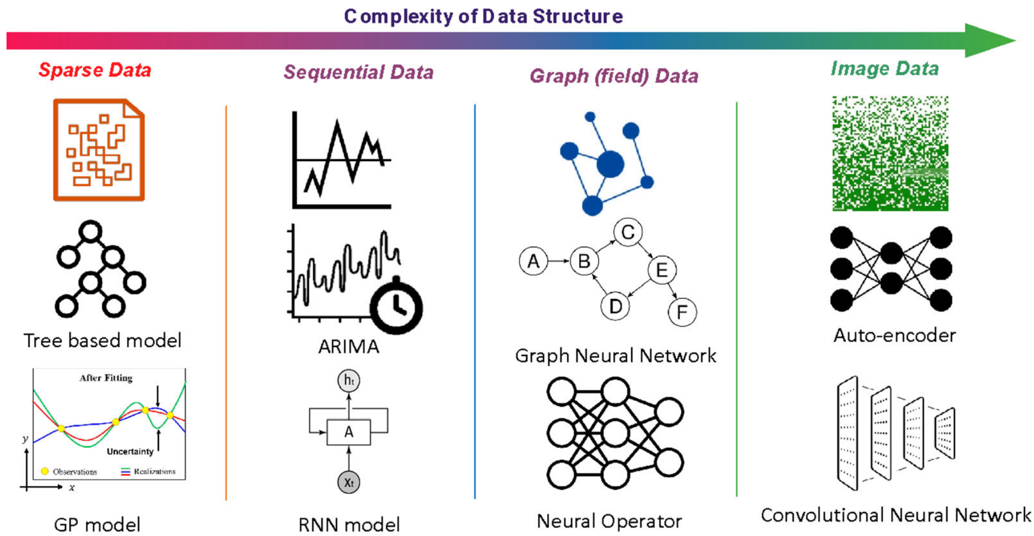

Figure 3. Representation of various data structures categorized by complexity, ranging from sparse data to image data. Sparse data include network diagrams and multi-dimensional scatterplots, demonstrating minimal information points. Sequential data are represented by time-series graphs and flow diagrams, emphasizing temporal progression. Graph (field) data illustrate interconnected nodes and network relationships, highlighting structured interactions. Lastly, image data display dense pixel arrays, ideal for visual content analysis. GP = Gaussian process; RNN = recurrent neural network; ARIMA = autoregressive integrated moving average.

In addition to the traditional ML techniques, generative models present a promising opportunity for enhancing the adaptability and flexibility of digital twins in manufacturing (Kusiak 2020; Regenwetter, Nobari, and Ahmed 2022). Models such as generative adversarial networks (GANs) and autoencoder-based architectures have shown significant potential in tasks such as data synthesis, anomaly detection and process optimization (Alfeo *et al.* 2020; Singh *et al.* 2020). GANs, for example, can be used to generate realistic synthetic data when real-world data are sparse or difficult to obtain, thus helping to train more robust models and fill gaps in the data for accurate predictions (Figueira and Vaz 2022). Similarly, autoencoders can be used for anomaly detection by learning the normal operating patterns of a manufacturing system and identifying outliers or unusual behaviours that may indicate equipment failures or process inefficiencies (Givnan *et al.* 2022). Furthermore, foundational end-to-end models, including generative pretrained transformer (GPT)-based models and diffusion models, can be adapted to digital twin frameworks to enhance their predictive capacity (Mu *et al.* 2024; Y. Sun, Zhang, *et al.* 2024). These models excel at processing complex, unstructured data and can help to improve decision making by providing actionable insights and adaptive control strategies. The integration of these generative AI models into digital twin systems can significantly enhance the scalability, precision and responsiveness of manufacturing processes, particularly in dynamic and unpredictable environments.

Figure 3 lists the ML models that can be used in digital twins according to the data structure of the information flowing (Bonaccorso 2018). To further enhance the integration of ML models into digital twin systems, it is important to consider the specific data structures being analysed. Different types of data, such as sparse data, sequential data, graph-based data and image data, require tailored ML approaches that can effectively process and interpret the information. Each data type presents unique challenges and opportunities for predictive accuracy and real-time decision making. Table 1 provides an organized overview of various ML models suited to each data type, offering a clear framework for selecting the right algorithm based on the nature of the data being processed. This comprehensive guide will aid in the optimal deployment of ML techniques within digital twins, ensuring robust and efficient performance in manufacturing environments.

Table 1. Machine learning (ML) models categorized by data type for digital twin applications.

Data type	Examples of data	ML models
Sparse data	Network diagrams of manufacturing workflows (*e.g.* assembly line connections), multi-dimensional scatter plots of defect rates (*e.g.* defects at different machining stages), sparse matrices of sensor placements on machines	Decision trees (T. Chen and Guestrin 2016; Guo *et al.* 2021), random forest (V. Karkaria *et al.* 2023; V. N. Karkaria *et al.* 2023), gradient boosting machines (GBMs) (H. Lu *et al.* 2020), XGBoost (C. Lu *et al.* 2022).
Sequential data	Time series of toolpath coordinates (*e.g.* CNC toolpaths during machining), sensor readings of temperature/pressure over time (*e.g.* heat treatment), sequential logging of production cycle data (*e.g.* start and end times for each process stage)	Autoregressive integrated moving average (ARIMA) (Shumway and Stoffer 2017), recurrent neural network (RNN) (Yu *et al.* 2019), long–short-term memory (LSTM) (V. Karkaria, Goeckner, *et al.* 2024), hidden Markov models (HMMs) (Ghosh, Ullah, and Kubo 2019), temporal convolutional networks (TCNs) (H. Li and Qiu 2022)
Graph (field) data	Interconnected nodes representing robotic arms or automated systems (*e.g.* robotic assembly processes), process flow networks (*e.g.* routing of parts between machines), conditions at each processing node (*e.g.* material flow rates at joints)	Graph convolutional networks (GCNs) (Bonilla *et al.* 2022), graph attention networks (GATs) (L. Sun *et al.* 2023), neural operator (Kobayashi, Daniell, and Alam 2024), GraphSAGE (Y. Zhu *et al.* 2024), graph generative models (Regenwetter, Nobari, and Ahmed 2022)
Image data	Pixel arrays of thermal images during welding (*e.g.* infrared imaging for heat distribution), video frames of additive manufacturing processes (*e.g.* layer deposition monitoring), X-ray or CT scans of manufactured parts (*e.g.* defect detection in castings)	Convolutional neural networks (CNNs) (T. Wang *et al.* 2021), autoencoders (H.-X. Hu *et al.* 2023), UNet (F. Wang *et al.* 2024), variational autoencoders (VAEs) (Ramezankhani *et al.* 2024), generative adversarial networks (GANs) (Zotov, Tiwari, and Kadirkamanathan 2020), diffusion models (Jiang *et al.* 2024)

Note: CNC = computer numerically controlled; CT = computed tomography.

Incorporating these elements into digital twin systems transforms them into dynamic tools capable of supporting complex decision-making processes. By utilizing predictive models that are constantly updated and adapted, manufacturing operations can achieve higher efficiencies, minimize risk and respond more adeptly to unforeseen changes (Xi *et al.* 2024). This approach not only enhances the operational capabilities of digital twins but also ensures that they remain a valuable asset in the increasingly automated and data-driven landscape of modern manufacturing. The next subsection (Section 4.2) will investigate the capabilities of these ML algorithms to serve as foundation models for digital twin framework.

By selecting appropriate ML models tailored to specific data types, digital twins can efficiently process and interpret large amounts of complex information, laying the groundwork for more accurate predictions and decision making. These models not only support real-time adjustments but also enable long-term optimization in manufacturing processes. Building on this, the integration of foundation models offers a more comprehensive framework, providing digital twins with the ability to generalize across diverse scenarios and fine-tune their performance with minimal retraining.

4.2. Foundation model within the digital twin framework for manufacturing

The integration of foundation models into digital twin technology is increasingly necessary to meet the demands of manufacturing environments. As highlighted in recent research, foundation models offer a scalable and adaptable framework that could allow digital twins in future to continuously learn from multi-source data, manage uncertainty and improve decision making in real time (J. Wang *et al.* 2022). In the future, these models, trained on extensive physics-based datasets, will have the ability to generalize fundamental physical principles across various manufacturing processes, such as AM, making them crucial for maintaining robust system performance and operational efficiency. This

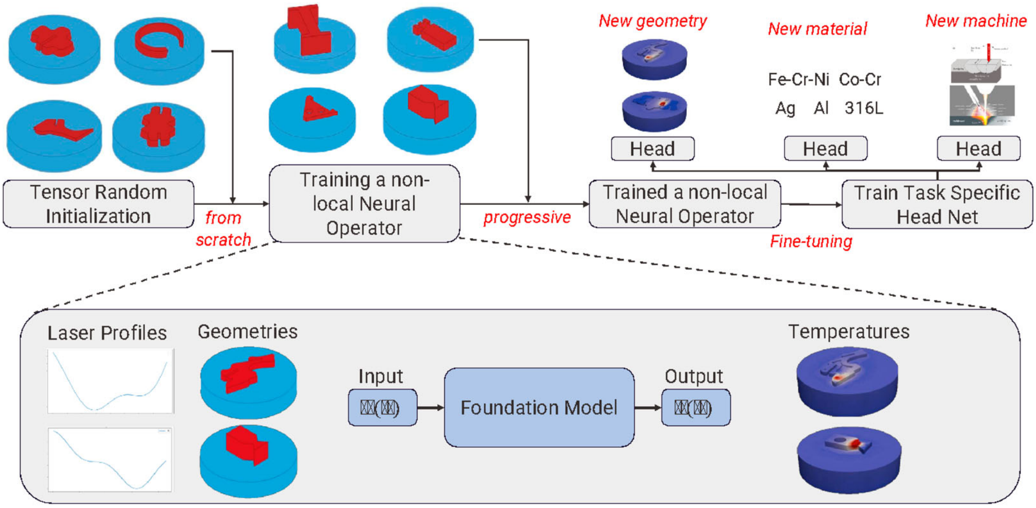

Figure 4. Training and application process of a foundation model tailored for manufacturing. It begins with tensor random initialization, and advances through stages where the model is trained from scratch to recognize and process various geometric shapes. The model is further adapted to new geometries, materials and specific machinery, demonstrating its versatility and capability for task-specific fine-tuning. The lower part of the diagram highlights the incorporation of a non-local attention operator, which enhances the model's ability to focus on significant features within the data, ultimately improving its accuracy and efficacy in real-world manufacturing applications.

transferability will allow foundation models to substantially reduce training time and computational resources, facilitating quicker deployment of digital twin systems.

The addition of foundation models into digital twin technology represents an advance in enhancing the capabilities of digital twins in manufacturing. Foundation models, which are large, pretrained models on vast datasets, provide a robust base that can be fine-tuned for specific tasks without the need for extensive training from scratch (Awais *et al.* 2023). In the future, by utilizing foundation models, digital twins will rapidly adapt to new manufacturing conditions or requirements, drastically cutting down the time and resources needed for model training. This swift adaptability will be vital for ensuring that digital twins stay relevant and effective in real-time decision making and process optimization. Figure 4 illustrates the anticipated flow of pretraining and fine-tuning foundation models across different manufacturing processes.

In addition, foundation models can be trained to capture shared physics, such as constitutive material laws, which makes it possible to transfer their application from one manufacturing process, such as AM, to another, such as welding or casting. This cross-domain adaptability not only reduces retraining costs but also facilitates the sharing of domain knowledge across different processes and materials, ensuring seamless scalability and applicability across diverse manufacturing systems.

Furthermore, by incorporating advanced learning techniques such as zero-shot learning, foundation models could be able to generalize to unseen tasks or manufacturing scenarios without requiring additional training data. This capability further enhances the flexibility of digital twins, allowing them to address novel challenges in dynamic industrial environments with minimal adjustments.

In terms of specific algorithms, transformer-based models (K. Han *et al.* 2023), neural operators (Kovachki *et al.* 2023), graph neural networks (GNNs) (L. Wu *et al.* 2022) and variational autoencoders (VAEs) (Zhai *et al.* 2018) are examples of foundation models that show promise in digital twin applications (Bommasani *et al.* 2022). Transformers, renowned for their effectiveness in handling sequential data, are ideal for modelling time-dependent processes in manufacturing settings, offering superior capabilities in understanding and predicting patterns over time (J. Wang *et al.* 2022).

VAEs, on the other hand, are useful for generating high-quality simulations. They can model the distribution of complex data, enabling digital twins to generate accurate and diverse scenarios for testing and optimization purposes (A. Wu and Deng 2023). GNNs excel at capturing relationships and interactions within complex systems, making them suitable for networked digital twin environments (Y. Liu *et al.* 2024). These algorithms help foundation models to effectively support the dynamic and multifaceted demands of digital twin technologies, enhancing their precision and utility in industrial applications. Furthermore, the integration of advanced models such as large language models (LLMs) has introduced new possibilities. For example, the development of unified LLM-based interfaces for robotics is beginning to inform the standardization of tasks in complex systems, offering a more generalized, adaptable framework for digital twins in manufacturing. These algorithms help foundation models to effectively support the dynamic and multifaceted demands of digital twin technologies, enhancing their precision and utility in industrial applications (Karamcheti *et al.* 2023).

4.3. Implementation of model updates and federated learning in digital twins

This subsection covers the methodologies used for updating ML models in digital twins through various modes, including offline, online and federated model updating approaches.

4.3.1. Offline and online model updates

In the model updating approach, periodic recalibration is critical for maintaining the relevance of digital twins as optimization tools. These updates allow the digital twin to incorporate the learned knowledge with the streaming data, ensuring that the prediction model remains trustworthy even as systems evolve. Model updates are particularly beneficial in manufacturing to enable adaptation to varying conditions, ensuring optimal performance and reducing downtime by continuously refining control strategies and processing plans based on the latest data.

The scope of model updating can be roughly divided into two types, offline and online model updating, depending on the updating frequency. Online model updating involves continuously refining a model in real time as new data become available during the manufacturing process. The main advantage is its ability to adapt to changing system dynamics, environmental conditions or uncertainties, making it highly suitable for applications in highly uncertain environments such as manufacturing or autonomous systems. This results in improved accuracy, responsiveness and resilience to disturbances. In applications such as AM, it helps the system to remain responsive to unforeseen changes (*e.g.* pores), facilitating robust and reliable operation. However, the downside is the increased computational burden, which can complicate deployment in resource-constrained environments. In addition, real-time updating requires careful design to avoid introducing instability or inaccuracies due to noisy data, emphasizing the need for robust model updating algorithms and efficient model validation techniques. Offline model updating, on the other hand, occurs after a batch of data has been collected, and is typically done as the manufacturing process is finished. The key advantage is that it allows for thorough, resource-intensive optimization and validation of the model without real-time constraints. This generally results in a more stable and well-validated model. For example, in AM, offline updates allow the digital twin to identify long-term issues, such as material degradation or production inefficiencies, that may not be apparent through real-time monitoring alone (Y. Li *et al.* 2024). The downside, however, is its lack of adaptability to new data, which makes it less effective in dynamic environments where the model's assumptions can quickly become outdated, reducing the model's long-term reliability. Several model updating methods are shared across online and offline model updating problems, while, in general, the online model updating requires more practical considerations, which hinder the application of some methods owing to their robustness and efficiency.

Estimating uncertain parameters for physics-based models has been discussed for decades, and it is still worth investigating how the implementation of this approach in manufacturing can be achieved for both offline and online model updating for digital twin systems (Nath and Mahadevan 2022;

Ouyang *et al.* 2020). It is often associated with physics-based or system identification models, represented by a manageable number of system parameters. In offline scenarios, parameter estimation can be achieved using a Bayesian calibration method (Jalal, Trikalinos, and Alarid-Escudero 2021) or maximum likelihood methods, providing a probabilistic estimate of parameters, or the estimation can be represented by the maximum *a posteriori* (MAP) of the distribution (Arendt, Apley, and Chen 2012; Aujla *et al.* 2018; Eweis-Labolle, Oune, and Bostanabad 2022; Kennedy and O'Hagan 2001; W. Li *et al.* 2016; Wei *et al.* 2022). On the other hand, in online processes with streaming data, the numerical efficiency and the robustness of the parameter estimation approach require rigorous evaluation, to determine whether there are enough newly collected data to perform a trustworthy model update. One popular approach for online model updating is the Kalman filter-based method, which not only assimilates the collected data with model prediction for state forecasting, but also updates the uncertain model parameters (Blanchard, Sandu, and Sandu 2010; Y.-P. Chen and Chan 2021; Cheng *et al.* 2023). However, the identifiability and robustness of simultaneously estimating multiple parameters online remain open questions, as most existing works do not fully address multiple solution scenarios, the realism of estimated physical parameters (*e.g.* the estimated parameters may lose their physical interpretation) and the required data quality for effective model updating at the same time. Moreover, these methods are likely to be numerically intractable when scaling up. Thus, ML methods are introduced in engineering applications to perform more efficient model updating for state predictions.

To utilize the ML model to capture the lack of knowledge while keeping the first-principles physics, hybrid models are widely used in engineering applications. In general, a physics-based low-fidelity model, usually in the form of a state-space model or a dimensional reduction model, will be obtained in advance to embed the first-principles physics. Further, as the system operation starts, an ML model, often known as a discrepancy model, will be trained and recursively updated to learn the discrepancy between the model prediction and the actual system response. Eventually, the fusion of the prediction of the physics-based model and the ML model will exhibit a more accurate prediction of the current system. Moreover, with a huge variety of candidate ML models, such as GP (Gardner *et al.* 2021) and neural networks (Kaheman *et al.* 2019), the implementation is straightforward, and the model will not usually encounter prediction stability issues, since the physics principles are still used as the backbone of the prediction and the discrepancy data are usually stationary. This method not only supports updating the model offline, but also is capable of real-time updating (Brynjarsdóttir and O'Hagan 2014; Maupin and Swiler 2020). However, one limitation of this grey-box approach is that, in some cases, the underlying physical model may not be accessible. Therefore, there is a need for the direct implementation of black-box data-driven models to identify the system directly.

As manufacturing systems are becoming more complex, to enable online and rapid predictions and decision making, the paradigm for model representation has gradually shifted towards data-driven models, mainly using deep neural networks (DNNs) (Bhuvaneswari *et al.* 2021; Gunasegaram *et al.* 2024). While DNNs can accommodate various types of data, capture highly nonlinear dynamics, scale up easily and offer high prediction speed, the updating of DNN models is relatively challenging (Pearlmutter 1989; Suykens, De Moor, and Vandewalle 1995). Mathematically, the updating or the fine-tuning of the model using the streaming data can use common model training methods such as stochastic gradient descent (SGD) to adaptively fine-tune the model (Bottou 2012; Tian *et al.* 2021). However, the underlying questions about model updating are how a model with many parameters can be updated efficiently and how accurate the model will be if it is updated using a relatively small amount of streaming data. To efficiently update the model, approaches such as low-rank adaptation (LoRA) and parameter efficient fine-tuning (PEFT) methods can be used to update the DNN model by focusing only on the important parameters (Ding *et al.* 2023; Z. Han *et al.* 2024; E. J. Hu *et al.* 2021). Moreover, one main issue that has been raised in the field of continuous learning is catastrophic forgetting, *i.e.* when an ML model rapidly loses previously learned knowledge upon learning new information through sequential learning. To avoid this, approaches such as regularization, dynamic architecture and memory replays can increase the generality of the model and its ability to handle the distribution shift of the data (Cossu *et al.* 2021; Mundt *et al.* 2023; Parisi *et al.* 2019). Even with these approaches, the integration of these methods, as well as the validation/certification to guarantee the trustworthiness of both online and offline updating of DNN, are still challenges, but they will play a critical role in digital twin manufacturing.

The transition from model updates to federated learning marks a significant shift in how data are processed and utilized in digital twin systems. While online model updating ensures that digital twins remain accurate and adaptive to real-time changes by continuously integrating new data, federated learning takes this a step further by decentralizing data processing and model training across multiple edge devices. This decentralization is crucial in modern manufacturing environments where data are generated at various distributed sites, and real-time decision making is required without the latency associated with centralized data processing. By employing federated learning in conjunction with edge computing, digital twins can perform model updates locally at each manufacturing site, ensuring both responsiveness and scalability. This approach not only enhances the accuracy of the digital twin but also optimizes resource utilization, allowing for efficient model updates across distributed networks. In the next subsection (Section 4.3.2), federated learning for model updates and its role in improving the efficiency and responsiveness of digital twin systems will be explored.

4.3.2. Federated learning for model updates

Federated learning, a decentralized ML approach, plays a crucial role in making digital twins more effective as optimization tools by allowing them to learn and adapt across multiple decentralized sources without requiring data to be sent to a central server. Instead, models are trained locally on edge devices and only the updates are shared, which ensures data privacy and reduces network bandwidth usage. This enhances the twin's ability to perform real-time optimization across distributed manufacturing sites. In manufacturing, federated learning is particularly useful when dealing with sensitive or proprietary data, such as process parameters in AM. By keeping the data local and only sharing model updates, manufacturers can optimize processes across multiple facilities without compromising confidentiality.

Edge computing, the practice of processing data closer to its source (at or near the edge of the network), further supports this by enabling the analysis and processing of data directly at manufacturing sites. This is critical in manufacturing environments where real-time decisions need to be made based on physical data, such as in monitoring the melt pool in AM processes. Immediate processing of these data at the edge allows for rapid adjustments in digital twins (Qi *et al.* 2018). By deploying edge computing solutions, data can be processed directly at manufacturing sites, which significantly reduces the latency typically associated with sending data to centralized cloud servers (Zhao *et al.* 2023). This proximity in data processing not only minimizes latency but also maximizes the responsiveness of digital twin systems, enabling them to handle real-time data processing and facilitate immediate decision making.

In a physics-based digital twin framework, this local processing is advantageous because it allows for the integration of first-principles physics models with real-time data from sensors. For example, in AM, edge devices can use shared physical models related to material behaviour under heat, enabling more accurate predictions and control of the process in real time. This physics-based approach, combined with federated learning, allows the digital twin to continuously refine its models across different manufacturing sites, improving overall system performance. This capability is crucial for maintaining continuous and efficient production lines, where even minor delays can lead to significant disruptions and losses. Edge computing allows for a more robust and responsive digital infrastructure, capable of supporting high-frequency decision-making processes that are essential in modern manufacturing environments (Dhungana *et al.* 2021).

In the context of edge computing, specific algorithms are optimized for such environments to ensure efficient data processing and decision making at the edge of the network (Aujla *et al.* 2018). For instance, lightweight machine learning (LightML) algorithms and stream processing frameworks are particularly suitable for edge computing scenarios (Sliwa, Piatkowski, and Wietfeld 2020). LightML

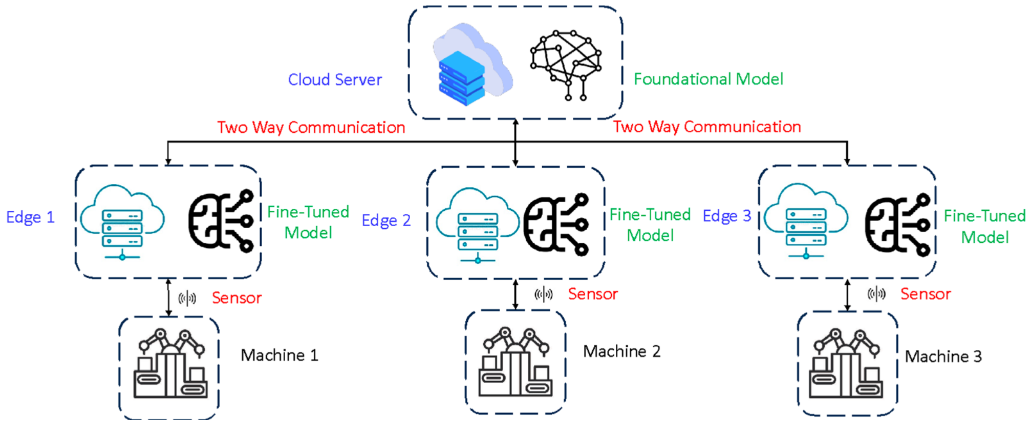

Figure 5. Illustration of federated learning, showing a distributed edge computing architecture featuring three edge devices, each integrated with sensors and a fine-tuned model, communicating bidirectionally with a cloud server that hosts a foundation model. This set-up facilitates real-time data processing and synchronization, using local computation at the edge for efficiency while centralizing model management for robustness in the manufacturing digital twins.

algorithms are designed to require fewer computational resources, making them ideal for the limited processing power available at edge devices (Dutta and Bharali 2021). Similarly, stream processing frameworks, such as Apache Kafka and Apache Flink, are designed to handle real-time data streams efficiently, processing incoming data on the fly without the need for batch processing (Raptis and Passarella 2023). These technologies are integral to implementing edge computing in digital twin systems, enhancing their ability to provide timely insights and enabling automated responses directly from the manufacturing site, thereby optimizing operational efficiency and productivity.

Figure 5 illustrates a distributed edge computing architecture featuring three edge devices, each integrated with sensors and a fine-tuned model, communicating bidirectionally with a cloud server that hosts a foundation model. This set-up facilitates real-time data processing and synchronization, employing local computation at the edge for efficiency while centralizing model management for robustness in the manufacturing digital twins.

In addition, edge computing enables the integration of advanced physics-based simulations directly at the source, which is particularly important for real-time adjustments in processes such as AM. For example, real-time monitoring of a melt pool in AM can use lightweight algorithms to adjust parameters such as heat distribution on the fly, ensuring optimal layer formation without the need for sending vast amounts of data back to a central server for analysis. Furthermore, edge computing enhances the scalability of digital twins by distributing computational loads across multiple edge devices. This decentralized processing is essential for large-scale manufacturing operations, where continuous, high-frequency decision making is required to maintain production quality and efficiency. By combining these lightweight and scalable technologies, digital twin systems become more robust and capable of handling the demands of modern manufacturing environments.

Section 4.4 will explore the critical role of uncertainty quantification within digital twins, a key component that enhances their predictive accuracy and reliability, particularly under complex and variable manufacturing conditions (Peterson *et al.* 2024). Effective uncertainty management, incorporating both epistemic and aleatoric aspects, ensures that digital twins can operate not just reactively but proactively (Hribernik *et al.* 2021). By integrating advanced statistical methods to manage and quantify uncertainties, digital twins are equipped to offer more robust decision-making tools that enhance operational efficiency and minimize risks (V. Karkaria *et al.* 2021; Wagg *et al.* 2020). This strategic approach to uncertainty management directly complements the real-time capabilities facilitated by edge computing, establishing a seamless operational workflow from data acquisition to decision implementation in the manufacturing process.

4.4. Uncertainty quantification

Verification, validation and uncertainty quantification (VVUQ) are crucial components in the development of robust digital twins, particularly in complex manufacturing environments, where variability and unforeseen conditions can significantly impact production outcomes (Wagg *et al.* 2020). The first step involves differentiating and quantifying the two main types of uncertainties: epistemic (model uncertainty) and aleatoric (inherent randomness) (Hüllermeier and Waegeman 2021).

Epistemic uncertainty arises from a lack of knowledge or data about the system being modelled. It can be reduced as more information becomes available or as the model's fidelity improves (Nannapaneni and Mahadevan 2016). In the context of digital twins, epistemic uncertainty can be addressed through techniques such as Bayesian networks, which provide a framework for incorporating prior knowledge and evidence to update the probabilities of hypotheses as new data become available (Vassilev, Laska, and Blankenbach 2024). This method allows digital twins to continuously learn and adapt their models, thereby gradually reducing epistemic uncertainty. Another effective approach is the use of ensemble methods, where multiple models or simulations are run with slightly different initial conditions or parameters to explore a range of possible outcomes (H. Wu and Levinson 2021). This helps in understanding the sensitivity of the system to various inputs and refining the model based on collective insights from the ensemble. In addition, incorporating quantile loss functions in these models can help in quantifying the uncertainty in predictive modelling by estimating the conditional quantiles of the outcome, which is particularly useful in risk management, where extreme values (tail risks) are of interest (Dong, Chan, and Peters 2015).

Aleatoric uncertainty, on the other hand, refers to the variability that is naturally present in the system owing to inherent stochastic processes or unpredictable external factors (Bevan 2022). For example, various sources of uncertainty, such as joint clearance and transmission errors, may negatively impact the robotic manipulation for manufacturing applications (K.-L. Li, Tsai, and Chan 2018; Tsai and Chan 2019). This type of uncertainty cannot be reduced through additional data or improved modelling techniques, but can be effectively quantified and managed (Walker *et al.* 2003). Monte Carlo simulations are particularly adept at handling aleatoric uncertainty (Karanki *et al.* 2017). By running a large number of simulations with random inputs drawn from probability distributions representing the uncertainty in those inputs, digital twins can estimate the probability of different outcomes, providing a robust basis for risk assessment and decision making. Techniques such as probabilistic programming also allow for the explicit modelling of randomness, and can integrate seamlessly with digital twins to simulate and predict under conditions of uncertainty (Kapteyn, Pretorius, and Willcox 2021). Applying quantile regression within this framework can further enhance the handling of aleatoric uncertainty by focusing on the conditional quantiles of the distribution of outcomes, thus providing a comprehensive view of possible scenarios and their associated risks (Sabater *et al.* 2021).

Validation and verification complement uncertainty quantification by ensuring that the digital twin accurately represents the real-world system and that the simulations are solving the correct equations accurately (Wright and Davidson 2020). Validation involves comparing the model predictions to real-world observations to ensure that the model is capturing the relevant physics and operational dynamics (Oberkampf, Trucano, and Hirsch 2004). Verification, on the other hand, is focused on assessing whether the model is implemented correctly and operates as intended under varying conditions (Vairo *et al.* 2023). Together, these steps build the foundation for a reliable digital twin, enhancing its predictive capabilities and robustness (Bécue *et al.* 2020).

Figure 6 illustrates a comprehensive framework for managing uncertainties in manufacturing processes through the integration of physical and digital systems. It shows how material and manufacturing variability, along with environmental and aleatoric uncertainties, impact the physical system, which includes manufacturing processes and pre-processes. These physical aspects are continuously monitored and adjusted via a model-based control, which uses updated surrogate model parameters influenced by sensor noise and model uncertainties (Hong *et al.* 2020). The digital system side depicts

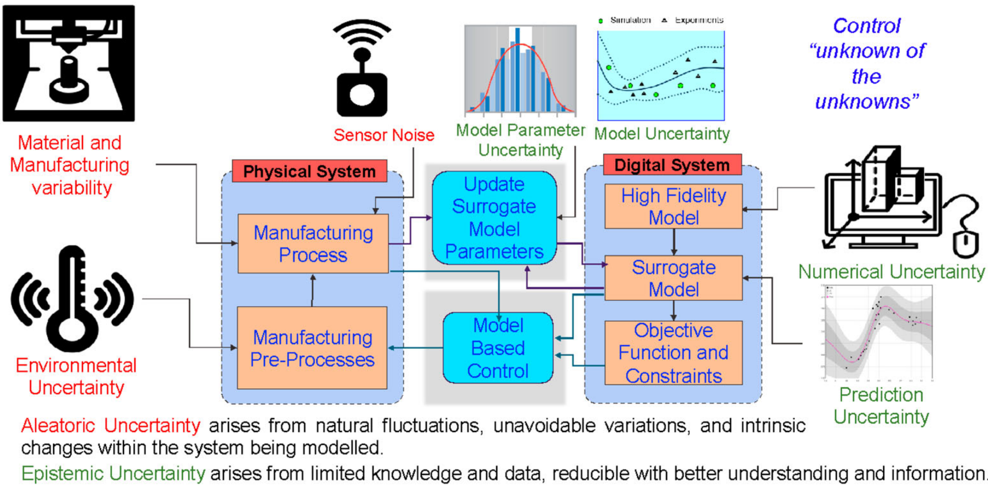

Figure 6. A comprehensive framework for managing uncertainties in manufacturing processes by integrating physical and digital systems, highlighting how variability and uncertainties are addressed through continuous monitoring, model updates and simulations.

the use of high fidelity and surrogate models to handle numerical and prediction uncertainties, aiming to control the 'unknowns of the unknowns' in the system through simulations and experiments.

Using these advanced statistical methods, including the integration of quantile loss functions, digital twins can provide more accurate risk assessments and robust forecasting models. They can help manufacturers to effectively manage potential variability and complexities in production processes, ensuring better preparedness and response strategies. Digital twins equipped with capabilities to quantify both epistemic and aleatoric uncertainties can optimize operations not only under normal conditions but also under various scenarios of uncertainty, enhancing the resilience and efficiency of manufacturing systems.

While digital twins can handle real-time uncertainties and operations through advanced statistical techniques, there is also a critical need for comprehensive offline optimization. Offline methods play a complementary role by allowing for deeper exploration of system behaviour, model refinements and control strategies without the constraints of real-time processing. These optimizations ensure that digital twins are well prepared for various operational scenarios, using historical data and simulations to enhance performance and reliability.

5. Solutions for offline optimization techniques for digital twins frameworks in manufacturing

Offline optimization plays a crucial role in the design, validation and updating of digital twin systems by using past data and computationally intensive methods to improve system performance without real-time constraints. Offline optimization is typically used for refining control strategies, tuning model parameters and improving predictive accuracy. The key optimization techniques described in Sections 5.1–5.6 are widely applied in this domain.

5.1. Genetic algorithms (GAs) in manufacturing and digital twins

GAs are evolutionary optimization techniques inspired by the process of natural selection. These algorithms are essential in digital twin frameworks, especially for offline optimization, where comprehensive system performance improvements require the processing of large datasets and the adjustment of complex variables in multi-dimensional spaces. They are particularly effective in complex, multi-dimensional search spaces typical of manufacturing processes, where multiple variables and constraints must be optimized. In manufacturing, decisions often involve both toolpaths and processing conditions, making GAs particularly suitable for handling mixed-variable problems. In the context of digital twins, GAs are valuable tools for optimizing process parameters, improving system performance and ensuring robust model updates to mirror real-world systems accurately. The iterative nature of GAs makes them ideal for offline optimization, as they can fine-tune model parameters and evolve solutions without the pressure of real-time decision making. This ensures that digital twins can provide optimized strategies before implementation in physical systems. For instance, GAs can simultaneously optimize discrete variables (*e.g.* toolpath selection) and continuous variables (*e.g.* temperature, pressure and feed rate), making them versatile for mixed-variable optimization in manufacturing. They are particularly beneficial in scenarios requiring long-term optimization, where historical data can be analysed to enhance production outcomes. A study integrating digital twins and GAs demonstrated the ability to optimize production scheduling and workload distribution, significantly enhancing system efficiency by over 8.93% in real-time scheduling systems for manufacturing processes (Feng *et al.* 2021; Xuan *et al.* 2023). For example, the dynamic selection adaptive genetic algorithm (DSAGA) was applied in the solid-wood-panel production industry, where it improved process efficiency by optimizing the interaction between real-time monitoring systems and virtual models (J. Yang *et al.* 2024).

GAs are also powerful in handling multi-objective optimization, where competing objectives, such as minimizing energy consumption while maximizing product quality, need to be balanced. In digital twin-driven manufacturing, the non-dominated sorting genetic algorithm-II (NSGA-II) is frequently used to tackle such challenges. It efficiently explores trade-offs between objectives and helps decision makers to identify optimal compromise solutions (Y. Li *et al.* 2021). The key GA variants used in digital twins are:

(1) Standard genetic algorithm (SGA): Used in basic optimization tasks, SGA has been widely applied in industries such as computer numerically controlled (CNC) machining, where toolpath optimization is essential.
(2) NSGA-II: Widely used in multi-objective optimization scenarios, such as optimizing the balance between production speed and product quality in digital twin systems (J. Yang *et al.* 2024).
(3) Differential evolution genetic algorithm (DEGA): A variant of GAs that improves convergence rates in highly nonlinear problems. It has been applied in digital twins for robotic path planning and production line optimization (Goswami, Chakraborty, and Misra 2023).
(4) GA with surrogate-assisted constraint-handling techniques: Effectively handling constraints is challenging for GAs. By utilizing surrogate modelling techniques (*e.g.* classification for learning constraint boundaries), the optimizer can better explore candidates within the feasible region (de Paula Garcia *et al.* 2023; Tsai and Malak 2024; Tsai and Malak 2022a).
(5) Hybrid GAs: Combining GAs with other optimization techniques (*e.g.* local search algorithms), hybrid GAs are useful for optimizing both discrete and continuous variables in manufacturing (W.-K. Jung *et al.* 2021).

GAs play a critical role in optimizing process parameters, system performance and multi-objective trade-offs in manufacturing and digital twin systems. These algorithms enable more efficient, cost-effective and adaptable manufacturing processes, making them essential tools in modern industrial applications. In addition to GAs, other evolutionary algorithms, such as particle swarm optimization (PSO), also provide powerful solutions for optimization problems in manufacturing.

While GAs excel in solving complex optimization tasks by evolving a population of solutions over generations, PSO uses the collective behaviour of particles to explore the solution space. Both methods can be applied in digital twin frameworks to enhance process control and decision making by fine-tuning model parameters. GAs focus on maintaining diversity and ensuring global search capabilities, whereas PSO excels at converging rapidly to optimal solutions through collaborative exploration.

5.2. Particle swarm optimization (PSO)

PSO is a population-based optimization algorithm inspired by the social behaviours observed in swarming animals, such as birds and fish. PSO is highly effective for optimizing nonlinear, multidimensional problems, making it particularly useful in manufacturing systems, where processes involve numerous interacting variables. Within the context of digital twins, PSO can be applied to optimize processes, material properties and parameters, improving the predictive capabilities of ML models and enabling better process control and decision making.

In digital twin frameworks, PSO is employed to fine-tune the parameters of predictive models that simulate physical systems in real time. Digital twins require accurate representations of manufacturing processes, and PSO can dynamically adjust model parameters to minimize the discrepancies between the virtual twin and the actual system. This ensures that the digital twin remains an up-to-date reflection of the physical system. In addition, PSO has proven valuable in optimizing the co-design of material, process and geometric parameters, ensuring that all aspects of the manufacturing process are harmonized for maximum efficiency. PSO has been particularly valuable in optimizing energy management strategies, such as in plug-in hybrid vehicle systems, where real-time decision making is crucial (Chauhan and Barak 2022; Rehman, Ahmed, and Begum 2023).

For example, in a study that combined PSO with digital twin technology for energy management (Diz *et al.* 2023), the PSO algorithm was adapted to handle the complexities of the vehicle's real-time control system. This improved energy efficiency while maintaining performance under changing conditions (Vilar-Dias, Junior, and Lima-Neto 2024). Another key application of PSO in digital twins involves fault detection in industrial machines. By using PSO, the system can efficiently detect deviations from normal operations, providing real-time alerts and enabling predictive maintenance to reduce downtime (Vilar-Dias, Junior, and Lima-Neto 2024).

Over time, several variants of PSO have been developed to enhance its performance in specific contexts. The notable PSO algorithms used in manufacturing and digital twin applications include:

(1) Standard particle swarm optimization (SPSO): This is the foundation version of the algorithm, where particles represent potential solutions, and their positions are updated based on their velocity, which is influenced by both their best-known position and the global best-known position of the swarm. SPSO is commonly used in process parameter optimization for tasks, such as toolpath optimization in CNC machining and scheduling in manufacturing (Chauhan and Barak 2022).
(2) Self-adaptive particle swarm optimization (SAPSO): This variant enhances the standard PSO by allowing parameters such as acceleration coefficients and inertia weights to adapt dynamically during the optimization process. SAPSO has shown promise in improving the convergence rates for manufacturing processes that require quick adaptations to changes in the environment (G. Chen *et al.* 2006). For instance, in smart manufacturing, SAPSO has been applied to optimize multi-objective problems, such as reducing energy consumption while improving product quality (Lalitha *et al.* 2023).
(3) Multi-objective particle swarm optimization (MOPSO): In manufacturing systems, it is often necessary to optimize multiple conflicting objectives. MOPSO is designed to handle these problems, offering a set of optimal trade-off solutions. This has been successfully applied in digital twin-driven manufacturing systems, where objectives such as minimizing material waste and maximizing production throughput must be balanced (Coello Coello and Lechuga 2002; Mirjalili 2016).
(4) Jumping particle swarm optimization (JPSO): JPSO improves the exploration capabilities of the swarm by introducing random jumps, allowing the algorithm to escape local optima and

search for global solutions more effectively. This variant has been applied in complex manufacturing systems where the optimization landscape is highly nonlinear, making traditional PSO less effective (Rehman, Ahmed, and Begum 2023).

In the context of digital twins, offline optimization with PSO allows manufacturers to validate their operational strategies before applying them in real-world systems. By running detailed simulations, companies can anticipate potential issues, adjust parameters and optimize outcomes, ensuring that the digital twin is not just a reflection of the current system but a tool for continuous improvement. The use of PSO in offline settings further enhances the decision-making capabilities of digital twins by reducing the time and cost associated with trial-and-error testing in physical environments. However, while PSO excels at finding optimal solutions for nonlinear, multidimensional problems, it can sometimes converge prematurely to local optima, especially in highly complex optimization landscapes.

To address this challenge, simulated annealing (SA) offers a complementary approach. Unlike PSO, which focuses on rapid convergence, SA explores a broader solution space by allowing the system to accept suboptimal solutions early in the process, thereby avoiding being trapped in local minima. This makes SA an effective tool when applied in conjunction with PSO for more rugged optimization tasks within digital twin frameworks. Together, PSO and SA create a balanced offline optimization strategy that combines the fast convergence of PSO with the global search capabilities of SA, leading to more robust solutions in manufacturing systems. The next subsection (Section 5.3) explores how simulated annealing (SA) further enhances offline optimization by effectively navigating complex solution landscapes, making it a powerful addition to digital twin systems for tasks such as manufacturing line design, SCM and predictive maintenance.

5.3. Simulated annealing (SA) in offline optimization for digital twins

SA is a stochastic optimization technique inspired by the annealing process in metallurgy, where materials are heated and then slowly cooled to reduce defects and improve their overall structure (Suppapitnarm *et al.* 2000). The essence of SA lies in its ability to search for the global minimum of a function, particularly in complex optimization problems where numerous local minima exist (Moh and Chiang 2001). This makes SA an ideal candidate for digital twin systems, where optimization tasks often involve navigating a rugged solution landscape filled with local optima (Sit and Lee 2023).

In offline optimization, where real-time constraints are absent, SA proves particularly effective. Digital twins use historical data to simulate various configurations of a system before they are applied in the real world, and SA enhances this process by allowing for controlled exploration of suboptimal solutions early in the optimization process. This capability helps to avoid becoming stuck in local minima, thereby increasing the likelihood of finding a global optimum, which can optimize processes such as manufacturing line design, SCM or predictive maintenance.

For instance, in a digital twin-based system for biopharmaceutical manufacturing, SA has been successfully used to optimize lyophilization processes, enabling manufacturers to simulate the freeze-drying conditions and tune the parameters in an offline setting (Juckers *et al.* 2024). By allowing small, controlled 'uphill' moves during the optimization process, the system can explore a broader set of possible configurations, leading to more efficient process outcomes.

SA is particularly useful in cases where the optimization space has many conflicting objectives, such as in multi-stage manufacturing processes, where efficiency, cost and quality must be balanced. The following are examples of SA-based methods tailored for digital twin frameworks:

(1) Classical simulated annealing (CSA): This is the basic form of the algorithm, where the temperature is gradually lowered according to a predefined cooling schedule. CSA has been applied in process optimization within digital twins for industrial systems, such as optimizing machining parameters and production scheduling. In one study, CSA was employed to optimize the toolpath

generation in CNC machining within a digital twin model, ensuring better material utilization and minimizing waste (Delahaye, Chaimatanan, and Mongeau 2019).

(2) Hybrid simulated annealing (HSA): HSA combines the SA algorithm with other metaheuristic algorithms, such as GAs or PSO. This hybrid approach has been used in digital twin systems for AM, where complex material behaviour is simulated offline to optimize production strategies (P. Cao *et al.* 2019). By utilizing the strengths of both algorithms, HSA offers a more refined search space, improving convergence rates while maintaining SA's robustness in escaping local minima (Hedar and Fukushima 2002; Ramezanian and Saidi-Mehrabad 2013).
(3) Adaptive simulated annealing (ASA): ASA dynamically adjusts its parameters, such as the cooling rate and neighbourhood size, based on the problem's current state (Geng *et al.* 2011). This method has been applied to multistage process design, where complex interdependencies between various stages require highly adaptable optimization techniques. In digital twin systems, ASA has been used to optimize multi-objective tasks such as balancing production speed, quality and energy consumption (Geng *et al.* 2011).
(4) Parallel simulated annealing (PSA): In large-scale digital twin simulations, PSA distributes the optimization task across multiple processors, allowing for faster convergence and exploration of larger solution spaces. PSA has been used to optimize large-scale production systems and supply-chain networks, where computational efficiency is critical (Atiqullah and Rao 2000; Jayaraman and Ross 2003; Su and Hsu 1998). By running several SA processes in parallel, PSA allows digital twins to quickly find near-optimal solutions for complex manufacturing problems (Ram, Sreenivas, and Subramaniam 1996).

In the manufacturing industry, SA has been widely used for production line optimization, inventory management and machining process optimization within digital twins. For example, SA has been applied to optimize scheduling problems in manufacturing, where the goal is to minimize downtime and maximize throughput while ensuring that resource utilization remains balanced (Mousavi and Tavakkoli-Moghaddam 2013). The probabilistic nature of SA makes it well suited for such tasks, as it avoids becoming trapped in suboptimal solutions, unlike traditional gradient-based methods.

In design optimization**,** especially in the context of AM and material design**,** SA has been used to optimize material composition and design geometry (G. Liu, Xiong, and Rosen 2022). Digital twins can simulate the physical properties of different material configurations, and SA helps to identify the optimal configuration by efficiently navigating the high-dimensional search space.

In summary, SA is a versatile and powerful tool in the offline optimization of digital twin systems. By enabling 'uphill' moves and offering a controlled mechanism for exploring complex optimization spaces, SA allows digital twins to find global optima in challenging environments. This capability is especially crucial in manufacturing and design, where multiple objectives must be balanced, and the cost of real-time trial and error is prohibitively high. Various SA variants, such as HSA and PSA, enhance the algorithm's flexibility and speed, making it an indispensable part of modern digital twin frameworks. However, while SA excels at exploring a broader solution space, it may still require numerous function evaluations, which can become computationally expensive in high-fidelity digital twin simulations.

This is where Bayesian optimization (BO) plays a critical role in complementing SA by minimizing the number of evaluations required to find optimal solutions. Unlike SA, which explores the solution space more uniformly, BO builds a probabilistic model of the objective function, typically using a GP, to intelligently decide where to sample next. This reduces the computational burden in complex, nonlinear systems that require high-fidelity simulations, such as those found in digital twin applications for manufacturing. Section 5.4 will delve into the specifics of how BO can further optimize digital twin systems by reducing the computational costs associated with simulations, making it ideal for high-fidelity tasks such as production planning, machine calibration and design optimization.

5.4. Bayesian optimization (BO) in offline optimization for digital twins

BO is a highly effective method for optimizing functions that are expensive to evaluate, particularly when dealing with problems characterized by complex, nonlinear relationships, as is often the case in manufacturing and digital twin systems (Shahriari *et al.* 2016). BO builds a probabilistic model of the objective function, usually using a GP, to guide the search for the optimum by deciding where to sample next. In addition to GP, other models such as random forests, Bayesian neural networks (BNNs) and tree-structured parzen estimators (TPEs) can also be used to model the objective function (Altman and Krzywinski 2017; Olivier, Shields, and Graham-Brady 2021; Ozaki *et al.* 2022). These alternative methods are particularly useful in scenarios where the assumptions of GP are not suitable or when dealing with high-dimensional, complex spaces. This technique is especially beneficial for tasks that require a limited number of evaluations, such as when simulating high-fidelity digital twins of manufacturing systems (Snoek, Larochelle, and Adams 2012).

Digital twins simulate real-world processes and systems in a virtual environment, where optimization tasks such as production planning, machine calibration or design optimization require running computationally intensive simulations. BO excels in this context because it minimizes the number of evaluations needed by making informed decisions about where to explore next in the parameter space. This reduces the computational cost and time required to find optimal solutions, making it highly applicable to tasks such as optimizing manufacturing parameters for AM or toolpath planning (Deneault *et al.* 2021; V. Karkaria, Goeckner, *et al.* 2024; Rupenyan, Khosravi, and Lygeros 2021).

In AM, for example, BO has been used to optimize laser power profiles and other process parameters in digital twin simulations, which, in turn, improve the mechanical properties of the final product. By using BO within a digital twin framework, manufacturers can test and fine-tune process parameters in a virtual environment before applying them to physical production, greatly enhancing efficiency and reducing costly trial-and-error experimentation (Ben Amor *et al.* 2024). Several specific BO algorithms have been applied to optimize digital twins in manufacturing settings:

(1) Gaussian process-based Bayesian optimization (GP-BO): This is the standard approach, where the objective function is modelled as a GP. GP-BO has been widely applied in manufacturing process optimization, such as machining or material testing within digital twins. For example, GP-BO is used in the optimization of heat treatment processes, enabling precise control over material properties based on simulated outcomes in the digital twin (Binois and Wycoff 2022).
(2) Bayesian optimization for time-series process optimization (BOTSPO): This variant is especially relevant in systems where the processes evolve over time, such as in time-series predictions within AM. BOTSPO uses a reduced-dimensional process profile generator to dynamically optimize process parameters, ensuring that the system adapts efficiently to changing conditions. In laser energy deposition, for instance, BOTSPO identifies optimal laser power profiles to achieve the desired mechanical properties in real time (V. Karkaria, Goeckner, *et al.* 2024).
(3) Multi-fidelity Bayesian optimization (MFBO): In digital twins, running high-fidelity simulations can be expensive. MFBO enables the use of both low-fidelity (approximate) and high-fidelity (accurate but costly) evaluations to speed up the optimization process. By incorporating both types of data, MFBO reduces the computational load while still converging on an optimal solution (Kandasamy *et al.* 2017). This approach is especially useful in complex multistage manufacturing processes, such as automotive assembly or aerospace component manufacturing (Y.-P. Chen *et al.* 2024).
(4) Bayesian inference for anomaly detection: Beyond optimization, Bayesian models are also used in fault detection and predictive maintenance in digital twin systems. By periodically sampling from the posterior distribution of a probabilistic model, Bayesian inference can detect anomalies in the system, such as deviations in machinery behaviour, and optimize maintenance schedules accordingly (Ruah, Simeone, and Al-Hashimi 2023).

BO's strength in digital twins lies in its ability to manage epistemic uncertainty–uncertainty arising from a lack of knowledge about the system. This is critical in offline optimization scenarios, where manufacturers need to optimize without the luxury of direct experimentation on physical systems. For example, in smart manufacturing, BO helps to optimize production workflows by using simulation data from digital twins to minimize energy usage while maintaining high product quality. This approach reduces operational costs and improves system resilience, making it a valuable tool for predictive design and process optimization.

In conclusion, BO is a powerful tool for offline optimization in digital twins, especially when dealing with expensive-to-evaluate functions and uncertain environments. Its applications in AM**,** machining and predictive maintenance have demonstrated its ability to improve process efficiency, reduce costs and enhance system robustness. By using advanced variants such as BOTSPO and MFBO, manufacturers can further accelerate their optimization efforts, ensuring that digital twins remain at the forefront of innovation and operational excellence. However, while BO excels in scenarios where evaluations are limited, it can be computationally intensive when dealing with highly complex models or when gradients of the objective function are available.

In such cases, gradient-based optimization methods, such as stochastic gradient descent (SGD) and adaptive moment estimation (Adam), provide a complementary approach by efficiently refining predictive models in digital twins. These methods are particularly useful when the gradient of the objective function can be computed, allowing for faster convergence in high-dimensional spaces. In offline digital twin settings, gradient-based techniques enable the optimization of parameters by minimizing errors between simulated and real-world measurements, thereby enhancing the accuracy of virtual models before their application in physical systems. The next subsection (Section 5.5) will explore the role of gradient-based optimization in digital twins, especially in manufacturing and design, where precise parameter adjustments are crucial for ensuring optimal performance without repeated real-world testing.

5.5. Gradient-based optimization in digital twins for manufacturing and design

Gradient-based optimization methods, such as SGD and Adam, are critical tools for optimizing ML models, as well as process, material and geometric design, particularly within the realm of digital twins used in manufacturing and design (Ahmadianfar, Bozorg-Haddad, and Chu 2020; Khan *et al.* 2021; Wormser *et al.* 2017; Yi, Ahn, and Ji 2020). These techniques rely on calculating gradients to iteratively update model parameters in the direction that minimizes the error or loss function. In the context of digital twins, gradient-based methods are employed to refine predictive models in offline settings, utilizing historical data to optimize systems without the need for real-time experimentation.

In the manufacturing sector, digital twins allow for precise simulation of production lines, machines and workflows, helping to optimize parameters before implementation in the physical world. Beyond ML, these optimization techniques can be extended to optimize material selection, geometric configurations and process parameters, ensuring that all aspects of manufacturing design are fine-tuned for maximum efficiency and performance. Gradient-based optimization, especially in offline scenarios, is crucial for updating these virtual models. This is because it efficiently finds the best parameters that minimize the difference between the digital twin's predictions and real-world measurements, improving accuracy and performance without having to repeatedly test on the physical system.

For instance, SGD and Adam are frequently used to optimize ML models embedded within digital twins, such as predictive maintenance systems that simulate equipment wear and tear. The gradient-based optimization algorithms help these systems to predict when failures will occur by minimizing the error in forecasts based on historical sensor data. Similarly, these methods are applied to co-optimize material properties, geometric designs and operational parameters in AM, ensuring that the digital twin provides accurate guidance for the physical manufacturing process. Adam is particularly suited to these tasks owing to its adaptive learning rates, which help to stabilize convergence even in highly noisy manufacturing environments (J. Chen *et al.* 2022; Nele *et al.* 2024).

Several gradient-based optimization algorithms have been tailored for use in digital twins:

(1) Stochastic gradient descent (SGD): The most basic form of gradient-based optimization, SGD is used to update model parameters based on a small batch of data. In digital twin applications, such as optimizing the performance of a production line, SGD allows for efficient updates by minimizing errors in predictive models used for process simulation (W. Yang *et al.* 2023).
(2) Adaptive moment estimation (Adam): A more advanced version of gradient descent, Adam calculates individual adaptive learning rates for different parameters based on both first and second moments of the gradient. In offline optimization of digital twin systems, Adam is used to fine-tune models predicting complex production variables, such as optimizing machining parameters for CNC systems (Kessels, Fey, and van de Wouw 2023).
(3) Root mean square propagation (RMSProp): Another variant of gradient descent, RMSProp adjusts learning rates based on the average of recent magnitudes of gradients. This is especially useful in digital twins for manufacturing, where complex, highly variable data from production lines need to be accounted for during optimization (Z. Wang 2024).

Gradient-based optimization is indispensable in product design within digital twins. For example, optimizing the design of components in aerospace or automotive industries involves adjusting a large number of parameters related to material properties, geometry and performance (L. Zhu, Li, and Childs 2018). Using algorithms such as SGD and Adam, digital twin systems can simulate how different design choices impact performance, allowing manufacturers to optimize designs before physical prototyping.

In energy optimization within production systems, gradient-based methods have been used to optimize energy consumption across multiple stages of production, helping companies to reduce costs and meet sustainability goals (S. Chen, Kaufmann, and Martin 2024; Jha *et al.* 2022).

In summary, gradient-based optimization methods such as SGD, Adam and RMSProp are crucial for the offline optimization of digital twin systems, particularly in manufacturing and design settings. By efficiently updating models based on historical data, these algorithms enable digital twins to optimize processes, predict outcomes and improve the overall performance of the system without the need for costly real-world trials. However, in more sensitive and fine-tuned manufacturing processes, where even small adjustments can lead to significant improvements, these methods may not be sufficient to ensure the necessary precision.

Trust region methods provide a solution to this challenge by focusing on optimization within a 'trust region' that surrounds the current solution. Unlike gradient-based methods, which may take larger steps in optimization, trust region approaches are designed to make incremental changes that improve accuracy without risking large deviations from the optimal path. In digital twin systems, trust region methods are particularly effective when optimizing highly sensitive parameters such as machine speed or material flow rates, ensuring that even the smallest adjustments lead to optimal performance without compromising the stability of the system. The next subsection (Section 5.6) will explore how trust region methods offer enhanced precision and control, making them an ideal choice for optimizing processes such as toolpaths in AM or control system tuning in complex production environments.

5.6. Trust region methods in digital twin optimization for manufacturing and design

Trust region methods are a class of optimization techniques that focus on iteratively solving a simplified model of an objective function within a defined trust region surrounding the current solution (Alexandrov *et al.* 1998). These methods are particularly useful in complex scenarios where high precision is necessary, such as when optimizing control strategies or process parameters in digital twin systems (Wen, Gabrys, and Musial 2022). Trust region methods are designed to find optimal solutions while avoiding large, uncontrolled steps that could lead to suboptimal results, making them ideal for fine-tuning in offline optimization processes common in digital twins (Bergmann and Cordier 2008).

In digital twin systems, trust region methods are used to optimize highly sensitive parameters, often associated with manufacturing processes that demand precise adjustments. These methods are frequently applied in control system tuning, where small adjustments to process parameters, such as machine speed, temperature or material flow rates, can have significant impacts on the performance and quality of production. By using a local approximation of the objective function, trust region methods enable accurate adjustments without causing large-scale disruptions to the system (H. Zhang *et al.* 2023).

For example, in AM, trust region approaches help to optimize toolpaths and laser settings within the digital twin, ensuring the quality of the printed material while minimizing defects such as porosity. In these applications, trust region methods balance the need for precision with computational efficiency, as they focus on adjusting parameters within a confined region of the solution space, making the optimization both robust and scalable.

Several trust region-based algorithms have been adapted and widely used in manufacturing and design applications:

(1) Trust region reflective (TRR) algorithm: This algorithm is commonly used to optimize parameters in systems with constraints, making it suitable for mechanical design optimization in digital twins. For instance, it is applied in aerospace component manufacturing, where the goal is to optimize material properties and structural integrity while adhering to stringent design constraints (Ahsan and Choudhry 2017).
(2) Levenberg–Marquardt algorithm (LMA): This hybrid method combines trust region principles with gradient descent and is highly effective in nonlinear least squares problems. LMA has been used to optimize control strategies in digital twin systems for robotic assembly lines, where nonlinearities in robot movement must be precisely modelled and controlled to reduce errors in real-world applications (Shawash and Selviah 2013).
(3) Dogleg trust region method: This method is well suited for optimization problems where computational resources are limited. It has been used in process optimization within digital twins for chemical manufacturing, where small adjustments in reaction conditions lead to significant improvements in yield and efficiency. The ability of the dogleg method to make rapid adjustments while maintaining accuracy makes it ideal for refining process parameters in iterative simulations (Lucia and Liu 1998).

The primary advantage of using trust region methods in digital twin-based optimization lies in their ability to ensure both precision and stability (Diouane *et al.* 2023). These methods enable engineers to fine-tune process parameters iteratively without risking significant deviations from optimal performance. In offline optimization scenarios, such as tuning ML models or refining energy consumption models in digital twins, trust region methods excel at maintaining a stable exploration of the solution space while converging towards an optimal set of parameters. Trust region methods offer a powerful, precise approach to optimizing complex manufacturing and design processes within digital twin frameworks. Their iterative nature ensures stability and prevents overadjustment, making them essential for applications where high precision and efficiency are critical. Whether optimizing material properties in AM or control strategies in robotic systems, trust region methods help manufacturers to employ digital twins to achieve higher productivity, lower costs and improved quality.

However, as manufacturing environments grow increasingly dynamic, offline optimization alone is not sufficient to keep pace with rapidly changing conditions. To ensure continued operational efficiency and responsiveness, online decision-making techniques must be integrated into digital twin frameworks. These techniques allow for real-time adjustments by processing vast amounts of live data from sensors and other sources, enabling immediate fine-tuning of production variables based on real-world conditions. The combination of offline optimization through trust region methods and real-time, data-driven online decision making creates a robust, adaptive system capable of maintaining optimal performance even as circumstances evolve. Section 6 will explore how online decision-making techniques further enhance the ability of digital twins to make real-time decisions by continuously updating models with new data, ensuring that predictions remain accurate and relevant in fast-changing manufacturing environments.

6. Solutions for online decision-making techniques for digital twins frameworks in manufacturing

This section discusses the importance of online decision-making techniques within the digital twin framework, particularly as manufacturing systems become more dynamic and data driven. The ability to make real-time decisions is crucial for maintaining optimal operational performance and responding to the ever-changing conditions of modern manufacturing environments. By using advanced algorithms, digital twins can process vast streams of real-time data from sensors and other sources, enabling immediate adjustments to production variables. This proactive approach helps to mitigate risks, minimize downtime and enhance overall efficiency. The integration of adaptive learning mechanisms and real-time process control techniques into digital twins allows manufacturers to fine-tune operations continuously, ensuring both short-term responsiveness and long-term system optimization. The following subsections (Sections 6.1 and 6.2) will delve into these key components, starting with adaptive learning mechanisms, which allow digital twins to evolve and improve based on new data.

6.1. Adaptive learning mechanisms

Adaptive learning mechanisms within digital twins represent an advance in the way these systems interact with and respond to changing manufacturing environments (Hribernik *et al.* 2021). By integrating continuous learning capabilities, digital twins can dynamically update and adjust their models based on new data continuously collected from sensors and other data sources (Rivera *et al.* 2019). This process allows digital twins not only to react to changes but also to predict future conditions and adjust operations proactively. The key to these capabilities lies in implementing advanced ML algorithms that can process and learn from data in real time, such as online learning algorithms which update the model incrementally as new data arrive (Nallaperuma *et al.* 2019). This continuous adaptation helps to maintain the relevance and accuracy of the digital twin's predictions, ensuring that the system stays aligned with the actual conditions of the manufacturing process and can effectively manage both expected and unexpected changes.

Figure 7 illustrates a controlled system designed to integrate both offline updates and online control for managing epistemic and aleatoric uncertainties, respectively. For offline updates, the system refines the predictive model through model updating and active learning methods for optimally querying the samples of simulations. The simulation data are used to update and calibrate the predictive model in MPC, which will be detailed in Section 6.2. For online control, it utilizes sensors and estimators to address real-time uncertainties (Saviolo *et al.* 2024). The integration of active learning, model updating and online control is able to adjust the system's responses even in the presence of disturbances and unpredictable actuation errors. Future work could combine residual policy learning with the MPC framework (S. Yang *et al.* 2020).

Moreover, adaptive learning mechanisms enhance the robustness of digital twins by allowing them to learn from anomalies and integrate this learning into future operations (H. Huang *et al.* 2021). For example, if a digital twin detects an outlier in the production process that could indicate a potential fault or inefficiency, it can analyse and learn from this incident to improve its predictive algorithms, thus enhancing future performance (Q. Lu *et al.* 2020). Techniques such as reinforcement learning

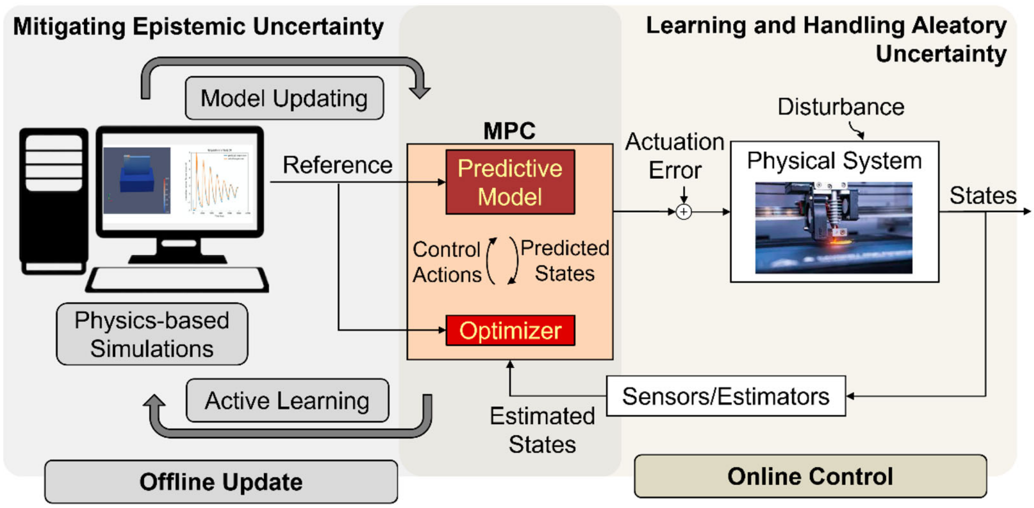

Figure 7. Conceptual diagram of a controlled system that integrates offline model updating with the interaction of physics-based simulations and online control with model predictive control (MPC).

(RL), where the model learns optimal actions based on reward feedback from the environment, are particularly useful in such contexts (Polydoros and Nalpantidis 2017). These models help digital twins not only to identify optimal operational strategies but also to continuously refine these strategies based on ongoing performance feedback (Bickford *et al.* 2020). This capability ensures that digital twins can keep evolving as intelligent systems, progressively improving their decision-making processes and operational strategies to optimize manufacturing outcomes continuously.

6.2. Real-time process control

6.2.1. Model predictive control (MPC)

Feedback control for manufacturing systems has been developed for decades, to improve controllability, performance and other key crucial metrics. For example, Liao *et al.* (2022, 2023) used proportional–integral controllers to control the melt-pool temperatures and depths in AM systems. However, those techniques lack the consideration of including constraints to enhance proactive capability and prevent defects from forming. MPC is an advanced feedback control method that solves in real time a finite-horizon optimal control problem at each sampling point, and is emerging as a powerful solution owing to its capability to effectively handle constraints (Schwenzer *et al.* 2021). Figure 8 shows that MPC can predict the future states and generate the control input with the moving horizon. Given the current state x_k and the reference trajectory $y^{ref}_{k:k+N} = [y^{ref}_k, \dots, y^{ref}_{k+N}]$, the problem can be generally formulated as:

$$J = \sum_{i=0}^{N-1} L(\hat{y}_{k+i}, y^{ref}_{k+i}, u_k) + L_N(\hat{y}_N, y^{ref}_{k+N}) \tag{1}$$

$$\text{s.t.} \quad \hat{x}_{k+i+1} = f(\hat{x}_{k+i}, u_{k+i}), \quad \forall i = 0, 1, \dots N-1 \tag{2}$$

$$\hat{y}_{k+i+1} = g(\hat{x}_{k+i}, u_{k+i}), \quad \forall i = 0, 1, \dots N-1 \tag{3}$$

$$\hat{x}_k = h(x_k) \tag{4}$$

$$c_i(\hat{x}_{k+i}, u_{k+i}) \le 0, \quad \forall i = 0, 1, \dots N-1 \tag{5}$$

$$c_N(\hat{x}_{k+N}) \le 0 \tag{6}$$

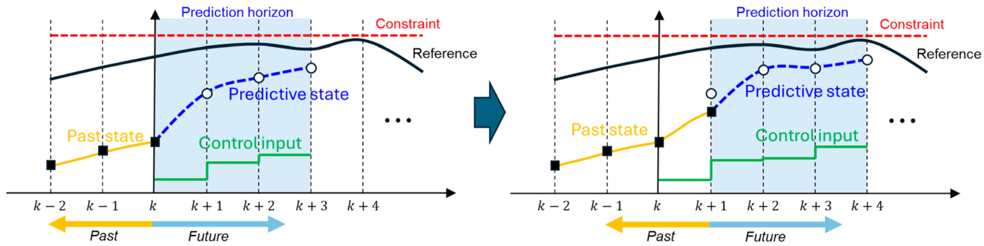

Figure 8. Illustration of model predictive control with moving prediction horizons.

where u_k is the control input at time k; L and L_N are the intermediate and terminal loss functions, respectively; $\hat{x}_{k+i+1}$ and $\hat{y}_{k+i+1}$ are the predicted state and output at time $k+i+1$, respectively; f and g are the predictive functions that describe the state evolution and the output, respectively; h is the state estimator; and c_i and c_N are constraint functions for intermediate state $\hat{x}_{k+i}$ and control input u_{k+i}, and the terminal state $\hat{x}_{k+N}$, respectively.

Although MPC offers advantages in handling multiple inputs and outputs with constraints, its computational complexity limits its application to systems with slow dynamics (Abughalieh and Alawneh 2019). Delay and latency issues cause the control actions to lag behind the actual system dynamics, potentially degrading performance or even leading to instability. MPC involves solving an online constrained optimization problem at every sampling point. The problem involves complex computations, making the optimization process time consuming, particularly for systems with fast dynamics requiring short sampling times in the order of milliseconds (Kozubik *et al.* 2024; Leuer and Böcker 2013). Parallel computing approaches offer a solution to address these real-time constraints by accelerating the MPC optimization process (Constantinides 2009; Soudbakhsh and Annaswamy 2013; Valencia-Palomo and Rossiter 2011). By dividing the problem into smaller subproblems or parallelizing the computations within the optimization algorithm, the computational burden can be distributed across multiple processing units, such as multi-core processors (central processing units), many-core processors (graphics processing units) or field-programmable gate arrays (FPGAs), enabling faster solutions and making MPC feasible for real-time control of systems with fast dynamics (Ferranti and Keviczky 2015; Kögel and Findeisen 2012; Nielsen and Axehill 2016).

In addition, building on the foundation established by adaptive learning mechanisms, MPC can be integrated as a model-based controller within the digital twin framework, especially in the realm of manufacturing (Omrany *et al.* 2023). This integration allows for meticulous planning and execution of operations, minimizing waste and enhancing efficiency by adjusting variables such as material inputs, speeds and temperatures in response to forecast changes in the production environment (Puigjaner *et al.* 2022).

Moreover, MPC within digital twins offers significant advantages when dealing with the complex, multivariable systems typically found in advanced manufacturing (Z. Huang *et al.* 2021). By continuously receiving updated data from the digital twin, MPC can adjust its predictive models and control strategies dynamically, ensuring optimal performance despite fluctuating demands and operating conditions (Xia *et al.* 2021). This dynamic recalibration is crucial for maintaining high levels of production quality and operational efficiency (Kenett and Bortman 2022). In addition, the forward-looking nature of MPC helps in anticipating future system states, thus providing manufacturers with a strategic advantage in proactively mitigating potential issues before they impact the production. The synergy between MPC and digital twins not only enhances the real-time decision-making capabilities but also bolsters the system's overall resilience, making it adept at navigating the complexities and variabilities inherent in modern manufacturing processes (Jin and Han 2024).

While MPC has been widely used to process control applications (X. Cao and Ayalew 2019; Y. K. Liu and Zhang 2014; Y. Liu, Wang, and Brandt 2019; Song and Mazumder 2011; Wehr *et al.* 2020), most of the related theorems have been developed based on the linear representation of the system.

This representation makes analysing the dynamic system easier and more interpretable, and provides rich theoretical support for ensuring recursive feasibility, constraint satisfaction and stability. Even the extensions of MPC, such as robust MPC (Mayne, Seron, and Raković 2005; Tsai and Malak 2023a), stochastic MPC (F. Li, Li, and He 2022; Tsai 2023) and adaptive MPC (K. Zhang and Shi 2020), are mostly established on the basis of linear assumptions. The fast-solving feature also allows the linear MPC to be executed in real-time practice. Although some methods attempt to convert black-box models into linear forms for the implementation of these tools using piecewise linearization, they are still performing a localized linearization and can only be used for short-horizon optimal control problems (S. Yang and Wan 2022).

6.2.2. MPC with ML

As ML and deep learning develop, they provide opportunities for modelling complex systems in a more manageable way (S. Chen, Billings, and Grant 1990; Ogunmolu *et al.* 2016). However, achieving high model accuracy while maintaining interpretability may not be practical for many model representations. Compared to models based on explicitly deriving the first principles of physics, deep learning models provide a straightforward approach to identify the systems accurately by capturing the nonlinear dynamics as well as the spatial and temporal dependencies between inputs. For example, sequence-to-sequence deep learning models have become popular for capturing long-term history and achieving faster predictions (M. Jung *et al.* 2023; J. Park *et al.* 2023). Some research has implemented RNN and LSTM as surrogates for process optimization (V. Karkaria, Goeckner, *et al.* 2024). However, there is still a lack of uncertainty quantification for deep learning methods that have been used for solving real-time control problems. Besides, attention-based methods, such as transformers, cannot offer access to interpretation of the underlying physics. In other words, the degree of interpretability may be reduced in exchange for accuracy, which raises concerns over rigorous proof as well as the real-time computational cost.

To address complexity and nonlinearity in engineering applications while maintaining the interpretable models, Koopman operators may be a game changer (Samak *et al.* 2024). As they can transform nonlinear dynamic systems into linear systems, linear control tools can be seamlessly applied in these settings (Korda and Mezić 2018). However, when applied to high-dimensional systems, Koopman operators can become computationally expensive owing to the need for a large number of observables to accurately represent the dynamics. The Koopman framework also scales poorly as the system's complexity increases. In recent years, with the maturation of autodifferentiation in computational methods, accurate gradient calculations can be performed while implementing the gradient-based optimizer, which significantly reduces the number of iterations using finite difference (M. Jung *et al.* 2023). Despite this, it remains extremely challenging to effectively handle constraints, especially in solving real-time optimization problems. A typical solution to this challenge is to reformulate a constrained optimization problem into an unconstrained optimization problem using penalty and barrier methods (Drgoňa *et al.* 2022; Zeng, Zhang, and Sreenath 2021). However, these methods do not guarantee that a feasible solution will be obtained, and require exhaustive hyperparameter-tuning tasks. Plausible solutions include adding stopping criteria to terminate the process within a certain time and reducing the control frequency to give MPC sufficient solving time.

A potential solution for enabling real-time MPC using a deep learning model as the surrogate is to convert the MPC from a solving problem into a predicting problem using policy learning models, also known as explicit MPC or neural network-based optimization (NNBO) (Alessio and Bemporad 2009; Bemporad *et al.* 2002; Gonzalez *et al.* 2023; Tsai and Malak 2021, 2022b, 2023b). The idea is to train a surrogate model that imitates the solving process of MPC to reduce the real-time computational effort, rather than repeatedly solving optimization problems. For example, differentiable predictive control treats the MPC objective with the penalized constraints as the training loss and uses derivative information to train an explicit control policy (Drgoňa *et al.* 2022). Since the training of the control policy is an end-to-end learning process, and represents the policy as a form of knowledge, it provides promising connections with RL methods (Q. Han, Boussaid, and Bennamoun 2024;

Karg and Lucia 2021), which will be detailed in Section 6.2.3. For example, the learned policy can be used as an initial sample for the RL agent to reduce the cost of exploration (Karg and Lucia 2020). While this method learns the policy directly by model prediction, the quality of the learned policy relies on the sampling of the training data, requiring comprehensive samples to adequately cover the entire state space (Ahn *et al.* 2023). Furthermore, formulating the policy in an end-to-end manner may neglect the physics and decision-making processes of MPC, making interpretation nearly impossible and limiting the applications in reality. In conclusion, the integration of real-time MPC with digital twins presents a compelling strategy for optimizing manufacturing performance and material properties. By using the predictive capabilities of MPC within the dynamic, virtual environment provided by digital twins, manufacturers can achieve higher precision in process control, reduce waste and enhance product quality. However, the choice of model representation and its compatibility with MPC are crucial factors that impact the overall effectiveness of this integration. Balancing model accuracy, interpretability and uncertainty quantification is essential, as is considering the computational demands of real-time optimization. As the field continues to evolve, the development of innovative approaches, such as policy learning and NNBO, holds promise for overcoming current limitations and pushing the boundaries of what can be achieved through this powerful synergy of technologies.

6.2.3. Reinforcement learning

Regarding policy learning, RL is a popular ML framework in which an agent learns to make sequential decisions by interacting with an environment to achieve a defined objective (Bușoniu *et al.* 2018; Shakya, Pillai, and Chakrabarty 2023). The agent selects actions, receives feedback in the form of rewards or penalties, and iteratively refines its decision-making policy based on this feedback. The learning process strategically balances exploration and exploitation to identify an optimal policy that maximizes cumulative reward over time. RL can play a pivotal role in advancing digital twin technology for manufacturing applications by developing intelligent agents capable of optimizing complex processes and handling large-scale systems (Y. Liu *et al.* 2022; K. T. Park *et al.* 2021; Xia *et al.* 2021; W. Yang *et al.* 2023). There are many examples that successfully apply RL techniques, such as Q-learning, deep deterministic policy gradient (DDPG), deep Q networks (DQNs) and proximal policy optimization (PPO), into manufacturing, supply chains or smart cities (Cakir *et al.* 2024; Khdoudi *et al.* 2024; Martin and Oger 2022; Y. Sun, Van, *et al.* 2024). RL algorithms, in conjunction with digital twins, enable the creation of virtual representations of physical manufacturing systems that can be used to train agents in a risk-free environment, allowing for the exploration of various manufacturing strategies and learning from both successes and failures without impacting the physical system (Y. Liu *et al.* 2022; Xia *et al.* 2021). Furthermore, the integration of RL with digital twins addresses key challenges in modern manufacturing, such as optimizing production schedules, enhancing real-time adaptability to dynamic conditions, and enabling predictive monitoring to prevent faults and ensure system resilience (Khdoudi *et al.* 2024; K. T. Park *et al.* 2021). However, one of the main challenges is that RL typically requires a large number of interactions with the environment to learn effective policies, which may lead to slow convergence and time-consuming training processes (K. T. Park *et al.* 2021).

To address the limitations of RL, particularly the high sample complexity and slow convergence, researchers have explored several strategies to enhance its efficiency and applicability within digital twins for manufacturing. For example, the concept of imitation learning offers significant advantages and drastically reduces the amount of data and resources required for data collection (Hussein *et al.* 2017; Le Mero *et al.* 2022; Norouzi *et al.* 2023). To begin with, the agent can be trained and initialized using the state-to-action pairs collected by human operations or controllers through behaviour cloning. By observing and mimicking expert demonstrations, the agent can be trained using supervised learning methods for behaviour cloning and precisely reproduce the demonstrated actions (Ahn *et al.* 2023). Furthermore, with good initialization, RL can be used to train the agent to continuously improve the policy, and eventually achieve performances beyond behaviour cloning. This method is particularly suitable for digital twin problems in which the environmental and operating conditions may vary along time or life cycles. With imitation learning, the agent can constantly adapt to unforeseen conditions based on the learned policy from the previous generation.

Another solution is multi-task policy learning, or task-dependent policy learning, which provides a data-efficient approach to generalize the learned policies across different tasks. In manufacturing, similar underlying physics across processes such as directed energy deposition and welding suggest that their control strategies should also share a common structure (D'Eramo *et al.* 2024; Hansen, Su, and Wang 2024; Marza *et al.* 2024; Vithayathil Varghese and Mahmoud 2020; Y. Zhang and Yang 2022). In addition, optimal control policies for different materials within a single process should reflect similar structural patterns, conditioned on material properties. Once the underlying physics across material properties and processing conditions have been learned and captured in the same latent space, the knowledge learned under different scenarios can be shared. The resulting learned policy is expected to yield better performance and generality by gathering and transferring knowledge from various tasks, with fewer training data being required from a single operating condition. Moreover, since the underlying physics is captured during task-dependent policy learning, it offers opportunities for the policy model to interpolate or extrapolate unprecedented materials and processes once their properties have been identified. Although this approach has not been widely applied to manufacturing problems, successful examples in robotics have shown great potential in various RL applications (Lan *et al.* 2019; G. Sun *et al.* 2021).

In addition to imitation learning and multi-task policy learning, residual policy methods can potentially improve sampling efficiency by using prior knowledge or existing controllers, reducing the costly and time-intensive data requirements typical in manufacturing (Silver *et al.* 2019). These approaches can also facilitate safer exploration, as they build on pre-existing control policies, minimizing the risk of errors during learning. In addition, residual policies can enable incremental adjustments rather than full replacements, making them suitable for conservative manufacturing environments (Abbas, Chasparis, and Kelleher 2022). Finally, they can be used in managing complex dynamics by compensating for model inaccuracies, supporting quick adaptation to changing conditions and allowing expert knowledge to be integrated through base controllers (C. Li *et al.* 2024). This combined approach can lead to robust, reliable solutions across varied conditions and may enhance interpretability, aiding its adoption in industrial settings. Nevertheless, there are some remaining challenges, such as increased complexity, dependence on the quality of the base policy, computational demands and potential stability issues, which may require careful implementation to maximize these benefits.

6.3. Co-design of materials and processes

Co-design integrates both offline and online optimization to enhance the decision-making process in manufacturing systems, bridging the gap between planned strategies and real-time adaptability. While offline optimization focuses on refining control strategies, tuning model parameters and improving the predictive accuracy of models, online optimization addresses the need for adaptive learning and real-time control adjustments based on evolving system dynamics. By combining these two approaches and the modelling techniques mentioned in Section 4, co-design enables a more comprehensive optimization framework in which offline strategies can inform online control actions, and real-time data can be fed back into refining the system's offline model, utilizing the control co-design (CCD) and multidisciplinary design optimization (MDO) formulations and algorithms (Allison and Herber 2014; Martins and Lambe 2013).

The co-design of materials, geometry and processes within a digital twin framework offers significant advantages for global manufacturing by enabling simultaneous optimization of these three domains (Boddeti *et al.* 2018; Kulkarni *et al.* 2015; J. Liu, Duke, and Ma 2016; S. Lu *et al.* 2019; J. Park *et al.* 2019; Querin *et al.* 2015). Traditional methods treat materials/geometric design and manufacturing processes sequentially, leading to suboptimal solutions or requiring many iterations to achieve results close to the system-level optimum (Allison 2014). Having constraints in the design problem can even increase the difficulty of searching for the optimum using a sequential approach (Tsai 2023). Co-design allows for a systematic approach that explores the interactions between material properties and process conditions. While some researchers have proposed topology optimization considering manufacturing uncertainty, part distortion and process variability in AM, a lack of process design still presents a challenge of maximizing product performance (da Silva, Beck, and Sigmund 2020; Komini, Langelaar, and Kriegesmann 2023; Mishra, Ayas, and Langelaar 2023). The mechanical performance of additively manufactured materials can be significantly improved by combining geometric design and toolpath planning (Kubalak *et al.* 2024).

Co-design can also foster customization and adaptability, allowing manufacturers to tailor both materials and processes to specific needs, which is critical in an increasingly on-demand and customized market. It also enhances sustainability by minimizing waste and energy consumption, aligning with global goals while improving cost efficiency. Digital twins accelerate this process by enabling rapid virtual testing and iteration, reducing the need for physical prototypes and shortening the time to market (Grieves 2023). Furthermore, co-design supports the resolution of complex manufacturing challenges, such as lightweighting in aerospace, by addressing multi-physics problems in a structured way, powered by AI and ML. Ultimately, integrating material and process co-design into digital twin frameworks enables manufacturers to innovate continuously, ensuring their global competitiveness and agility in an evolving market.

7. Conclusion

This article has explored the diverse and critical functions that optimization methods play within digital twin frameworks, focusing on real-time adaptability, long-term efficiency and decision making in manufacturing processes. Optimization techniques allow digital twins to facilitate real-time process adjustments, improve flexibility and scalability, and integrate AI to enhance predictive accuracy, making them indispensable in addressing the complexities of modern manufacturing environments. Furthermore, these methods support interdisciplinary optimization by harmonizing mechanical, thermal, control and other systems, which is essential for achieving high performance and efficiency in advanced manufacturing environments.

Through the implementation of various optimization strategies, digital twins have proven to be effective in managing uncertainty and mitigating risk across manufacturing systems. Optimization methods enable digital twins to navigate the inherent variability in manufacturing, providing stability and robustness through comprehensive scenario analysis and predictive maintenance capabilities. As such, digital twins can optimize resource utilization by balancing competing objectives, such as cost, quality and production speed, allowing for a holistic approach to process management. By integrating both online and offline optimization techniques, digital twins empower manufacturers to dynamically adjust to fluctuating demands and operational challenges, ultimately leading to continuous improvement and higher productivity.

In conclusion, optimization methods are foundational to realizing the full potential of digital twins in manufacturing. They ensure that digital twins remain relevant and effective tools for optimizing manufacturing systems, supporting adaptive decision making and maintaining operational resilience. As manufacturing processes grow more complex, the use of advanced optimization methods within digital twins will be key to achieving sustainable production models and enhancing global competitiveness. This article also identifies future potential directions in foundation models, federated learning and online–offline decision making within digital twin frameworks for manufacturing. The future of digital twins in manufacturing will undoubtedly rely on the ongoing development of sophisticated optimization techniques to meet the ever-evolving demands of this rapidly advancing field.

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Data availability statement

Data sharing is not applicable to this article as no new data were created or analysed in this study.

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