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Digital Twins: An Overview MDO Tools in the Design and Deployment of

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Abstract

Digital Twins (DTs) have received significant recent attention due to their transformative potential across various application domains, involving design, manufacturing, operations, and maintenance. They promise to enhance decisionmaking, enable predictive maintenance, improve operational efficiency, and manage complex systems. However, their design and deployment pose challenges, especially when moving beyond the widely used 'digital shadow' model prevalent in many industrial applications. This overview paper explores the concept of Digital Twins (DTs) and how they fundamentally represent a system-of-systems. The system-ofsystems framework captures how DTs interconnect multiple subsystems to function cohesively and adaptively. Multidisciplinary design optimization (MDO) tools and methods are considered critical in DT design and deployment. Special attention is required for issues such as modeling fidelity, uncertainty quantification, data analytics and integration, and real-time synchronization. Emerging tools involving artificial intelligence, machine learning, edge computing, and VR/AR-based human-machine interactions hold promise for exciting advancements in this technology.

Keywords: multidisciplinary design optimization, digital twins, domain decomposition methods, uncertainty quantification, augmented and virtual reality, optimization

1 Introduction

Digital twins [1-3] are virtual replicas of physical objects, systems, or processes, created using traditional modeling and simulation approaches but where the model is continuously augmented by real-time data obtained from the physical entity. They enable monitoring, analysis, and optimization of their real-world counterparts, providing insights and predictive maintenance. The concept may be traced to an effort at NASA to develop a digital mock-up of the Apollo 13 to study scenarios for a space rescue mission [4]. Michael Grieves is largely credited for coining the phrase in describing its use in product life cycle management and later in a 2014 white paper [5,6]. In 2012 Glaessgen and Stargel [7] offered what is perhaps the most broadly accepted definition of a digital twin as *"…an integrated multiphysics, multiscale, probabilistic simulation of an as-built vehicle or system that uses the best available physical models, sensor updates, fleet history, etc., to mirror the life of its corresponding physical twin."* This description sets it aside from other terms such as a 'digital model' or a 'digital shadow' that are sometimes confused for digital twins. While a digital model can be created without any exchange of data between the physical entity and the model, digital shadows do sometimes incorporate data from the physical asset to improve or augment the digital counterpart [8]. A two-way flow of information between the physical asset and its digital counterpart is what separates a digital twin from a digital shadow (Figure 1a). A five-dimensional digital twin model has been proposed (Figure 1b) that shows the flow of data and control to and from the digital twin. The role of both online and offline optimization in the continual training and feedback from the digital twin is highlighted in this figure.

Figure 1a. Digital Shadow & Twin Figure 1b. Five-dimensional Digital Twin

The global digital twin market size was estimated at US\$16.75B in 2023 and was projected to grow at a compound annual growth rate (CAGR) of 35.7% from 2024 to 2030. DTs have been pursued successfully in several applications in manufacturing, asset monitoring, and in enhancing operational efficiency.

Examples of such developments include the work done at GE Aerospace in creating a Digital Twin of a jet engine [9], a near exact digital replica of the physical asset. Onboard sensors and cloud connectivity allow for data collection on the physical asset that is continuously transferred to the digital copy, updating that model as necessary. This virtual twin replicates the performance of the physical engine, allowing for continuous monitoring of performance and enabling predictive maintenance, resulting in enhanced reliability and productivity by managing the aircraft downtime.

Manufacturing accounts for a major share of the global digital twin market [10]. By creating virtual models of equipment, the floor layouts, and of production processes, workflows and operations can be optimized in the digital space. Siemens Numerical Control in China that produces production systems, drives, and motors, implemented a digital twin that allowed them to consolidate three factories into one, reducing facility costs through optimized space and reduced wastage. Mars, the food and pet care company, used a digital twin to optimize it's supply chains and boosted uptime at 160 factories.

Another application directed at operational efficiency is a digital twin of the entire city of Shanghai [11]. In addition to detailed modeling of landmark structures and buildings, data from satellites, drones, and other sensors was used to generate digital copies of other buildings, water bodies, open spaces, and transportation network. This model is open to continuous enhancement as additional data is collected and is of immense value for those seeking to improve services, plan new developments, optimize building systems, and design for improved traffic flow. The digital twin assists in both operations and future designs and developments

It is abundantly clear that for each of the examples, the effort and resources required to create the digital twin are significant. Additionally, digital twins can be designed at various levels of complexity, starting with a replica of an individual part or component. For instance, various components of a jet engine could be individually modeled as a digital twin and be used to perform health checks, plan maintenance or replacement, or even redesign the component for improved performance. At the next level, these component twins can be integrated to replicate a physical asset, such as a jet engine (Figure 2).

Figure 2. Component twins combined into an asset twin

The asset twin, which models the integrated functioning of the components, provides information about the asset's performance and condition to predict failures and suggest interventions for repairs or replacements. It can also be used to simulate new operating scenarios that could redefine component or asset design. Different asset twins would then integrate into a system twin, replicating the performance of the system. For

example, a digital twin for the jet engine could be combined with the twin for the fuel control system to form the powerplant system, allowing for assessments of performance and potential failure points, including control actions to optimize the maintenance schedule.

When designing a jet airplane, for example, the performance of the airplane can be modeled by the digital twins of its many subsystems. How these subsystems interact with one another must be considered when integrating them to create a digital model of the airplane. This represents a complete system in of itself. However, the airplane must be acquired, scheduled for operations to yield optimal payback, and maintained for maximal reliability and use, but at least cost. Each of these tasks is a separate system for which digital twins can be created. Combining these individual systems into a single system (one can also integrate this into an air transportation system model) results in a system-of-systems digital twin that replicates the real-world operating environment, providing a potent tool to test, predict, and even design this collection of systems.

Figure 3. A Simple System-of-Systems Representation of Digital Twins

Such an application of digital twin technology in design, manufacturing, and operation/sustenance requires considerable investment of resources to realize the full potential – digital twins must be thought of as a parallel asset [12] that much like its physical counterpart, must go through the phases of conceptualization, structure or architecture formalization, detail design, deployment and working under a prescribed maintenance and update cycle (Figure 3). While current practices focus on developing this digital asset once a physical asset is available, there may be merit in pursuing these two assets in parallel, particularly if longer service lives are in play.

The field of Multidisciplinary Design Optimization (MDO) or Multidisciplinary Analysis and Optimization (MDAO) developed out of a recognition that optimal configuration and design of practical engineering systems involves multiple disciplines, and that the interactions between these disciplines must be fully considered for maximal impact. Additionally, these interactions must be included formally and based on sound mathematical formulations. Success in the adaptation of nonlinear programming methods in structural optimization [13-15] led to early efforts in expanding those approaches to multidisciplinary design problems and reviews of these developments are available in [16,17]. The need to formally account for interactions among disciplines has brought focus on approaches to decompose such system design problems into smaller interconnected subsystems, either purely on disciplinary lines or taking advantage of any obvious hierarchy in the analysis and design problem. These decomposed subsystems may be optimized sequentially, inparallel, or both, depending upon the topology of the resulting decomposition [18].

Meaningful implementation of these approaches requires attention in some key areas, including a) decomposition strategies and architectures; b) efficient methods of analysis for design (efficient physics-based models, approximate or surrogate models, data based models); c) optimization algorithms (mathematical, heuristic); d) optimization strategies (all-in-one, simultaneous analysis and design, sequential linear programming, etc.); e) uncertainty quantification and uncertainty based design (uncertainty quantification in analysis, probabilistic design); f) Data handling and visualization; and g) human-machine interactions. Emerging tools of artificial intelligence and machine learning have had their own impact in many of these areas. AI deployed within digital twins assists through analysis of data, in the creation of predictive models, and identifying potential problems in the physical system. Similarly, AR and XR tools help merge the real and physical world, allowing the user to interact with the physical world. Some of these issues will be discussed in later sections of this paper. A schematic of these areas of research is presented in Figure 4.

Figure 4. MDO: Areas of Research Focus

Tools for data management and handling are an important consideration in the design and development of digital twins. Data collected from sensors on physical assets is of high dimensionality. In many instances, data is in the form of a time series [19,20], could be multi-modal and/or obtained from multiple sources. There is also uncertainty in data collection (sensor errors) and data transfer processes (transmission losses) that must be managed [21-23]. There are challenges related to preprocessing and preparing this data for machine learning applications.

Subsequent sections of this paper examine various aspects digital twin design, with a special focus on how approaches developed in the context of multidisciplinary design optimization can provide answers to challenges of a high-dimensionality data intense environment, deeply coupled interactions, and a computationally demanding problem.

2 Implementing Digital Twins

As stated in the preceding section, the design of a digital twin for any realistic physical system could proceed in a manner similar to designing the physical asset. A conceptual or preliminary design must be developed to satisfy high-level system functionalities. This conceptual design proceeds to a more detailed design phase, and the resulting system tested and verified before deployment. It is no surprise, therefore, that advancements in MDO methods are directly applicable to a structured development of digital twins.

2.1 Architecture & System Decomposition

At the outset of the digital twin building process, it is crucial to identify the characteristics of the system under consideration, whether it is a single complex system or a system-of-systems. Typically, the digital asset is built from multiple digital twins representing simpler components or subsystems, and it is important to clarify the flow of information among these twins to adequately account for interactions.

MDO methodology involves the collaborative use of computational tools and algorithms to evaluate and refine designs across multiple interconnected domains. A key ingredient in this approach are methods for decomposing systems into smaller, more manageable subsystems to tackle complex design challenges effectively. These include hierarchical decomposition [24], where systems are broken down into nested levels of subsystems; collaborative optimization [25], which allows parallel optimization of subsystems while coordinating their interactions; and analytical target cascading [26,27], which systematically propagates design targets from the system level to subsystems and components, ensuring alignment with overall system objectives. When applied to digital twin design, the design variables would be the model parameters that need to be optimally selected for the model response to duplicate the behavior of the physical asset. The latter serves to define the objective and constraint functions in the optimization.

These architectural frameworks are important not only for design optimization, but also underscore the importance of understanding the inherent structure of the analysis under consideration, as to how this analysis is coupled or linked together to direct the flow of information in the overall system. Both issues are important in the design and deployment of digital twins. Both formal and heuristic methods have been proposed in the MDO literature in this context – two of the more widely used methods, the Design Structure Matrix and Directed Graphs are briefly discussed in subsequent sections

2.1.1 The Design Structure Matrix (DSM): The coupling among sub-systems is well captured by a DSM [28] diagram. This tool provides a systematic way to represent and analyze the interdependencies between subsystems, facilitating efficient coordination and integration in multidisciplinary problems. Figures 5a-b show a hybrid coupled system and its generic DSM representation. There are six subsystems that are in play and the flow of information is shown by the arrows going into and emanating from the blocks. The DSM shown in Figure 5b has several cells, where each cell indicates the presence (X) or absence (blank) of a dependency between the subsystems.

Figure 5a. Topology of Coupling Figure 5b. DSM - Representation of Coupling

In designing multidisciplinary systems, the ordering or grouping of analysis in the subsystems becomes important as a means of controlling computational costs. For example, it becomes computationally expensive if the completion of analysis in A is contingent on receiving information from F and then iterating further to convergence. On the other hand, if F does not need information from other blocks to compute the output, it would be more efficient to move the execution of F closer to the execution of A.

When the number of subsystems or components included in the DSM are nominal, the reordering of executions can be performed based on a visual inspection. As this number increases into hundreds, more formal methods involving optimization techniques have been deployed for the purpose [29]. A highly cited approach is the Design Manager's Aid for Intelligent Decomposition (DeMaid), first released by NASA in 1989 to assist a designer understand the interactions among different components of a large complex system [30,31]. The original version included functionalities for minimizing the feedback couplings, grouping activities into iterative sub-cycles, and sequencing the design activities. DeMaid has been enhanced with addition of optimization algorithms to optimize the sequence of processes within each iterative sub-cycle based on time, cost, and iteration requirements [32].

2.1.2 Directed Graphs: Directed graphs [33], also known as digraphs, present another tool for representing the coupling within a system. In the context of multidisciplinary design optimization (MDO), a directed graph consists of nodes and directed edges, where each node represents a component or a subsystem, and each edge represents a dependency or interaction between subsystems. A directed graph represents general one-way relationships between nodes and can include cycles, illustrating various types of directional relationships without specific context. A dependency graph is a specific type of directed graph, that provides more structured and context-specific information about the order and precedence of tasks or modules.

Formal graph theoretic methods have been considered in the design literature [34-36]. The approach includes constructing a directed graph that describes all possible interconnections between a set of coupled analysis tools. Graph operations are then to reduce this densely connected graph to a fundamental problem graph that describes the connectivity of analysis modules required to solve a specific system-level design problem. In the context of digital twins, this approach could be used to provide the best architecture of the digital twin for a required functionality.

The use of formal methods such as the ones described above would be invaluable in identifying the flow of information through the system of systems and could clearly identify the input and output from each component or subsystem digital twin that constitutes this assembly. It also aids in the process of integrating these digital twins into a digital model that represents the entire system. An analysis of weights of trained backpropagation neural networks has been used as another approach for identifying topology of decomposition in coupled multidisciplinary problems [37,38].

2.2 Modeling and Simulation

MDO methodology is based on the availability of mathematical/computational models that represent the system behavior and are coupled with optimization algorithms to search for optimized designs. Similar modeling techniques are foundational to the development of digital twins. Generation of such models involves a variety of methods that combine data acquisition, computational techniques, and domain-specific knowledge. Geometric models are quite central in digital twin development, particularly in modeling layout of factories and production processes. To reflect the behavioral response of physical assets however, the types of models most typically used include physics-based models that rely on the fundamental principles of physics to simulate the behavior of these systems [39]. Data driven models are also widely implemented that use historical and real-time data to generate

and update models [40]. These approaches involve the use of statistical and machine learning methods to develop predictive models. A short discussion of these models is presented next.

2.2.1 Solid Modeling: Geometric modeling using CAD (Computer-Aided Design) techniques involves creating precise mathematical representations of objects, which can be visualized and manipulated in a virtual 3D space. This process of creating realistic and precise geometric models is critical in digital twins for manufacturing and assembly, where process flows and human machine interaction can be modeled, simulated and optimized. Both machines and their operating environment can be represented by such geometrical models. Popular software packages such as AutoCAD, SolidWorks and Catia have been used [41] alongside gaming engines such as Unity3D [42] and Unreal Engine [43] for these tasks. Development of such models is a time intensive process and in many instances the trend is one where major equipment manufacturers are now providing digital models as a service to the consumer.

LiDAR (Light Detection and Ranging) techniques have been deployed to create geometric models; this involves scanning physical environments with laser pulses to capture precise spatial data that is then processed to generate detailed 3D models representative of the real-world asset. Examples of this approach include creating the model of an environment in which a human interacts with a robotic arm [44] to optimize the robot movements for safe operations. Another example is an application of laser scanning to quickly map the geometry of large structures [45]. A disadvantage the use the laser scanning approach is the inability to model internal spaces in physical objects.

2.2.2 Physics-Based Models: Where appropriate, physics-based models drawn from fundamental principles and well-known governing equations are used to simulate the different aspects of the physical system, from component models to subsystem/system models. Mechanical models based on classical mechanics principles can be used to analyze stress, strain, deformation, and kinematics in structures and materials. Likewise, the Navier-Stokes equations can be used to analyze flow patterns or pressure distribution in fluids, or Maxwell's equations used to model electromagnetic fields, and chemical kinetics principles used to predict reaction rates. Multiphysics models integrate multiple physical phenomena to provide comprehensive simulations of complex systems, such as combining fluid dynamics, heat transfer, and chemical reactions to simulate combustion engines. Each type of model is crucial for accurately representing and predicting the behavior of real-world systems in digital twin applications.

Finite element (FEA) and finite difference (FD) methods provide numerical approaches to solve complex partial differential equations (PDEs) that describe physical phenomena and comprise the mainstay of physics-based models for digital twins. Several commercial tools are available that implement these approaches and that integrate well with CAE and solid modeling software. ANSYS Mechanical and ANSYS Fluent, ABAQUS, & MSC Nastran are some examples that have been used extensively. Combination of these methods have been deployed in in MDO problem solutions such as wind-turbine modeling [46] and aeroelastic design [47]. These early successes and extensive user experience has led to a natural adaptation into the design of digital twins for applications such as stress analysis of a ground vehicle suspension [48], in the wear analysis of a machining tool [49], and in the analysis of a battery cooling system [50].

In MDO problems, models of different fidelity are deployed at various stages of the design process. The design of a new jetliner begins with conceptual design, moves to preliminary design before detailed analysis and design is performed. The design is then tested and validated before deployment in practice. As shown in Figure 6, analysis models of different fidelity are deployed at each stage of the design process.

Figure 6. Schematic of the Design Process

Similarly, in designing and deploying digital twins, it is important to consider the trade-off between computational speed and accuracy that must be built into a model. In doing so, however, it is important to bear in mind that even high-fidelity models have inherent errors that may result from incompletely modeled or misunderstood physics of the problem; discretization errors are always a concern when a continuous problem is represented by a discrete assignment of nodes or elements. The added consideration in designing digital twins is that there is a bi-directional flow of data between the digital and physical assets. This creates opportunities for using data to tune model parameters but requires that the number of such parameters be limited because of constraints on the number of sensors in the physical asset. Design of such models becomes an embedded optimization problem that links the physical and digital assets in ways not encountered in traditional MDO problems. In most digital twin implementations, physics-based models are kept at intermediate fidelity and only a limited set of model parameters are considered in the online tuning. This is also desirable in the context of computational time for model execution – real time response from digital twins is required in many applications. MDO methods have focused on developing surrogate models for analysis to reduce the computational time for optimization [52-54]. These developments translate directly to development of data-driven models for digital twins.

2.2.3 Data-Based Models: Data-based models are particularly useful in complex and dynamic environments, such as modeling industrial IoT applications, healthcare, or complex engineering systems. In such applications. traditional physics-based models may be insufficient (even lacking) or too computationally intensive. If data can be generated from a physical asset for different combinations of input parameters, surrogate models can be generated using techniques such as linear regression, polynomial response surfaces [55,56], Kriging [57,58], generalized Bayesian methods [59], support-vector machines [60,61], and radial basis methods [62]. Data to train these surrogate models can also be generated from expensive physics-based simulations; the trained models would then be used in digital twins in lieu of the physics-based models. AI and machine learning (ML) methods have also been used to develop surrogate models. It is worthwhile to state that all these techniques have been extensively explored in the context of MDO problems.

Linear regression offers the simplest surrogate model characterized by very low computational resource requirements. However, it offers limited applicability in modeling nonlinear interactions and polynomial response surfaces are more widely used in data-based models. They too are usually applied to model less complex behavior spaces, with the ability to capture the main effects and first-order interactions. These models generally work well for low dimensionality problems. Another widely used technique is based on a Gaussian process model. This technique, commonly known as Kriging, represents the function to be represented by a weighted superposition of known independent basis functions that define the trend of mean prediction The method does not require large numbers of parameters to be determined and works well for low dimensionality problems (parameters \sim 20 or less). The mathematics of the approach does not allow it to properly represent discrete parameter space. Support Vector Machines is another approach in modeling that partitions the parameter space into distinct clusters. Any new data point presented to this model results in a generalized output based on its proximity to the closest clusters [63].

In the domain of digital twins, data is used to either build surrogate models of a component, subsystem, or system behavioral response. Data can also be used to perform a system identification task for model development. With a trained model in place, sensor data can also be used to predict any behavioral change as may result from a damage or degradation in the system. The behavioral response models are generally obtained by tuning model parameters to minimize the error between predicted and expected response. System identification models follow a similar approach using sensor data to tune model parameters. The two classes of data-based models in digital twins are either ML models that include the surrogate models discussed above or statistical models. While the latter relies on the generation and tuning of a probability model, ML utilizes learning algorithms to find trends in large data sets [64] and an ability to generalize these trends for prediction. A useful way to look at various approaches [65,66] and tasks in model building is shown in Figure 7.

As shown in this figure, physics-driven surrogate models are obtained at the intersection of physics based modelling and big data solutions. Hybrid models are obtained from a combination of physics-based and data-driven models, and methods of data analytics.

Figure 7. Combination of physics-based and data-driven modelling (adapted from [66]).

2.2.4 Statistical Models: Digital twin design often involves handling time-series data, where statistical models play a crucial role. These models can identify patterns, relationships, and provide future estimates by mathematically representing the behavior available in the available data. Ranging from simple autoregressive models to more complex integrated moving average models, they offer a variety of options for analyzing and forecasting time-series data.

Autoregressive models [67] are frequently used for time-series analysis and forecasting. The method assumes that the time series is a linear combination of past observations. They are most useful for modeling univariate time series data. Historical data is used for training, with weighting coefficients determined that minimize the error between measured and predicted outputs. The method is useful for time series showing trends and patterns but the assumption of linearity between current and past values is somewhat limiting. The method requires large amount of data to make accurate predictions.

The moving average (MA) model [68] is another statistical technique used to model time-series. As opposed to the AR technique that uses past value to predict future values, the MA approach uses errors in past estimates (historical errors) to make future predictions. The coefficients of the model are determined by minimizing the difference between predicted and actual values. Current values are obtained as a linear average of past errors in prediction. The use of error variations in model building allows MA models to better account for irregular events. Like the autoregressive methods, they too suffer from a linearity assumption and require significant data for training.

The combination of the autoregressive and MA methods yields a powerful approach ARIMA (Auto-Regressive Integrated Moving Average) [69]) that is often used in digital twin development. ARIMA makes use of lagged moving averages to smooth time series data. The model consists of three distinct components – autoregression and moving average discussed earlier, and an integration component that replaces data values by the difference between the current data value and the previous value. The main advantage of ARIMA models is their ability to deal with non-stationary time series. There is considerable literature pertaining to the development of statistical methods for nonlinear system identification. The nonlinear autoregressive exogeneous (NARX) model [70] and the nonlinear autoregressive moving average model with exogeneous inputs (NARMAX) [71] have received significant attention.

Digital twins have also been used for predictive diagnostics and in this context, there has been focus on degradation modeling. Many statistical models have been proposed for modeling degradation and single/multiple failure modes. These include among many others, Markov and semi-Markov models [72,73], and accelerated life testing (ALT) models [74]. Markov models suffer from being designed to deal with abstract failure states that are difficult to correlate with measured sensor data for predictive use. Bayesian model updating schemes used in conjunction with Markov models are being explored to overcome some of these deficiencies [75].

Statistical modeling for digital twins remains a very active field of research and a comprehensive survey of this subject is included in [8]. These models have not been a subject of focus in MDO research but given their applicability to digital twins, this area will require increased attention.

2.2.5 Machine Learning (ML) Models: ML based models, in particular neural networks were adopted in MDO problems [76-78]. These early attempts focused on the use of multilayer backpropagation neural networks to create surrogate models for use in problems that were computationally intense, or where the optimization algorithms required repeated calls for function evaluations. The neural networks were trained on a set of input-output training patterns and the trained network used to predict output for an input pattern that was not part of the original training set. These trained networks were then connected to an optimization algorithm and responded to function evaluation calls from the optimizer as shown in the flowchart of Figure 8. Computational cost savings were realized during optimization, where exact analysis was not required whenever the optimizer needed information on the objective and/or constraint functions.

Figure 8. Trained Neural Network Surrogate Analysis Model for Optimization Other machine learning methods including support vector machines [79], Gaussian process regression [80], and backpropagation neural networks [81] have been used in digital twins for modeling degradation, system identification, and to replace physical models. Use of such models has enabled real-time predictions, an important requirement in digital twin applications.

The literature in machine learning has grown significantly since these early advances. Deep learning has emerged as an important new direction for research. Deep learning [82] involves networks with multiple hidden layers and a very large number of parameters to select during the training process. They can be configured to handle high dimensionality input-output training data and have the capability to accommodate datasets that may contain different data types, structures, or drawn from disparate sources. As with traditional ML methods, deep learning methods have also been used in digital twins for system identification, model degradation, and to create surrogate models of computationally intensive physics-based models [83-85].

Deep learning advancements have given rise to other neural network architectures that hold considerable promise for applications in MDO problems, and by extension, to the design and development of digital twins.

2.2.5.1 Physics Informed Neural Networks (PINN): Physics-Informed Neural Networks (PINNs) [86,87] are a class of neural networks that learn from the physics governing a particular problem. Unlike traditional neural networks that are trained strictly on data, a PINN leverages the underlying physics governing the system. This is particularly effective in problems where the physics may be described by partial differential equations (PDEs). A schematic of a PINN is shown in Figure 9 that illustrates how the training is based on a combination of limited numerical data but also a measure that indicates the satisfaction of the differential equation. More specifically, the learning of the network parameters is based on a minimization of the mean square error of numerical training data and a minimization of the residual of the partial differential equation for the system. While attractive for MDO problems as a surrogate model, this approach is particularly attractive for digital twins in problems where the number of sensors may be limited; this deficiency in numerical data is made up by ensuring a satisfaction of the physics of the problem.

Figure 9. Schematic of a PINN network

The approach is particularly elegant in that the derivative information required in the computation of the PDE loss function is automatically available in the backpropagation network computations. There are some issues, however, that may detract from the effectiveness of the approach. While first order derivatives are easily obtained in the computations, higher order derivatives and fractional derivatives require special treatment [88] that adds to the computational burden. Additionally, the loss function being minimized in the training comes from a combination of PDE residuals and numerical input-output data. Appropriate weighting of these terms is necessary to remove the bias. This notwithstanding, the approach has considerable promise for digital twin applications.

Other approaches falling into the category of physics-informed neural networks are data augmentation [89] and transfer learning [90] methods. In the former approach, the simulation data generated in the physics-based model is augmented with experimental observations to create an enhanced set of learning patterns for ML based learning. The transfer learning approach differs from the previous methodology in that the model is first trained using the data from the physics-based model. A fine-tuning operation is then invoked using experimentally recorded data.

2.2.5.2 Generative Adversarial Neural Networks (GANN): Generative Adversarial Networks (GANs) [91,92] are a class of neural networks designed to generate new data samples that resemble a given dataset. It has been used in the context of multiobjective design optimization for creating new optimal designs on the Pareto front [93]. As shown in Figure 10, the network consists of two principal components - a generator and a discriminator. The generator proposes new designs (also referred to as synthetic data), while the discriminator evaluates whether the data is real (based on its training on real data) or fake (produced by the generator).

Figure 10. Schematic of a GANN network

During training, the generator aims to produce increasingly realistic data to pass the discriminator test, while the discriminator strives to become better at distinguishing between real and fake patterns. This adversarial process continues until the generator produces high-quality data indistinguishable from the real dataset, making GANN a powerful tool for tasks like image synthesis, data augmentation, and super resolution. These networks have an important role in digital twins where additional data may be required to train surrogate models. When digital twins are designated for personnel training purposes (as in workforce development for machine operations), such networks could provide realistic data patterns representing new scenarios for consideration.

2.3 Uncertainty Quantification

A digital twin is a virtual representation of a physical asset that seeks to mirror its real-time state. As discussed in previous sections of the paper, the task requires the creation of digital models that simulate the behavior of the physical system and that must interact with real-time data to make useful observations, or to provide appropriate operational decisions. For there to be a level of confidence in using such systems, a systematic effort must be undertaken to quantify uncertainty in various elements of the digital twin design. Both aleatoric and epistemic sources of uncertainty [99] are endemic to such modeling efforts. The former refers to an irreducible form of uncertainty – it relates to things like uncertain material properties, manufacturing tolerances, uncertainty in load conditions, etc. Data recorded by sensors may have some inherent measurement errors or transmission of data may be subject to losses or corruption. These types of uncertainty are typically handled through an assumed probability distribution that would then allow for the computation of a level of confidence in any prediction. Epistemic uncertainty comes about from lack of knowledge such as may result from limited data, model definition, and or lack of knowledge that may result in poor assumptions. In ML-based models, this uncertainty can be reduced by making use of physics to enhance the prediction capabilities [87] (PINNs as described in the previous section).

The subject of uncertainty quantification is both important and is a highly researched area. Uncertainty or reliability-based design has been actively pursued in the context of MDO and is directly applicable to the digital twin problem. An extensive review of this field is beyond the scope of this paper. Nevertheless, some key approaches to epistemic uncertainty quantification in ML-based approximations in digital twins are included here for completeness.

There are non-probabilistic approaches to uncertainty quantification including fuzzy logic [94] and evidence theory [95]. Fuzzy logic provides a framework for handling uncertainty by allowing variables to take on a range of values with varying degrees of truth, rather than being strictly binary. By using membership functions and linguistic variables, fuzzy logic can effectively capture and process the inherent uncertainty in real-world situations, facilitating more robust decision-making and predictive analysis. Additionally, fuzzy logic can be combined with other computational methods, such as machine learning, to further enhance its capability for uncertainty quantification.

Evidence theory provides an alternative approach for defining uncertainty in terms of degrees of belief in events rather than fixed probabilities. In this framework, each piece of evidence is used to assign a degree of belief, known as a Basic Probability Assignment (BPA), to subsets of possible outcomes. A belief function is used to quantify the minimum degree of belief that can be committed to a subset of outcomes based on available evidence. Dempster's rule combines BPAs from different sources of evidence, updating the belief functions to reflect the aggregated evidence. The approach has been used for uncertainty quantification in [96].

In the context of digital twins, probabilistic methods have received greater attention for quantifying uncertainty in ML-based models [97-99]. These approaches are largely directed at quantifying epistemic uncertainty. Some of the more popular approaches are summarized as follows.

While computationally expensive and largely intractable for high dimensionality problems, Monte Carlo simulations have remained a popular approach due to their relative simplicity. Many random samples of uncertain parameters are used to run simulations and probability distributions obtained as the output. Another commonly used approach employs sensitivity analysis to evaluate how variations in input parameters affect the output of the model. By identifying the most influential parameters, efforts are focused on accurately characterizing these critical parameters. Techniques such as variance-based methods [100], Sobol indices [101], and local sensitivity measures are used in such an approach.

Gaussian Process Regression (GPR) is another technique that has been applied for uncertainty quantification [102], providing a flexible and non-parametric approach to modeling complex data. The approach assumes that the outputs of the training patterns follow a Gaussian distribution characterized by a mean function and a covariance function. The mean function typically starts as zero, and the kernel defines the relationship between points in the input space. The choice of kernel function is crucial as it represents assumptions about the function's smoothness, periodicity, and other properties. When new data is observed, the GP updates its beliefs about the function and computes a posterior distribution, which provides a mean function that predicts the expected output and a covariance function that quantifies the uncertainty around these predictions.

Bayesian Neural Networks (BNNs) [103] are an approach to quantify uncertainty in the predictions available from neural networks by incorporating Bayesian inference into neural network modeling. Unlike traditional fixed weight neural networks, each weight in BNNs is characterized by a distribution, typically Gaussian, with a mean and variance. During training, Bayesian inference is used to update the posterior distributions of the weights based on the observed data. This involves calculating the posterior distribution of the weights given the observed data. When making predictions, BNNs use the posterior weight distributions to generate multiple sets of outcomes. This distribution of predictions reflects the uncertainty in prediction. A drawback of the approach is in scaling to high-dimensionality input spaces.

Ensembles of neural networks have also been proposed [104] as another approach to quantify uncertainty. The process involves independently training several neural networks that have different architectures, weight initializations, and hyperparameters such as learning rate or batch sizes. The performance of each network is evaluated using the validation test data and the best performing networks are identified and their predictions aggregated using an averaging, weighted averaging, or voting (in classification problems) procedure. Ensembles tend to generalize better to unseen data compared to individual networks. They can mitigate the risk of overfitting, as the combination of multiple models smooths out the biases in an individual model. Ensembles can provide a measure of uncertainty in their predictions. The variance in the predictions of the individual networks can be used to quantify the confidence in the ensemble's output. A higher variance indicates higher uncertainty. Ensemble networks still incur a high computational cost due to the requirement of training multiple networks. This is a deterrent for their use in the real-time environment of digital twins.

Polynomial Chaos Expansion (PCE) [105] is a more advanced technique that represents the uncertain parameters as a series of orthogonal polynomials. PCE can efficiently propagate uncertainty through the model by approximating the model response as a polynomial function of the uncertain inputs. This method is particularly useful for systems with smooth responses and can significantly reduce the computational cost compared to Monte Carlo simulations.

Hybrid approaches that combine multiple UQ techniques are often employed to leverage the strengths of each method. For instance, coupling Monte Carlo simulations with surrogate models like PCE or GPR can provide a balance between accuracy and computational efficiency. The choice of UQ method depends on the specific characteristics of the system, the nature of uncertainties, and the available computational resources, making it essential to select the most appropriate approach for each application. An additional degree of complexity is introduced as one considers large dynamical systems and the need to quantify uncertainty in those systems in a computationally efficient manner [99].

3 Optimization for Digital twins

Optimization methods have a critical role in the design and deployment of digital twins. These methods are used to optimize digital twin parameters so that their predictions match those of the physical assets, to search through a space of possible decisions to find an optimal operational strategy, and to identify emerging problems in the physical system that need attention The latter refers to the application of optimization in predictive maintenance by forecasting potential failures and optimizing repair schedules, enhancing the reliability and lifespan of the physical systems. At the level of initial digital twin design, optimization is performed offline. Here, all aspects of system design are in play – system architecture, function approximations including uncertainty quantification, reliability-based design, decomposition of system and best coordination strategies for optimization, etc. Embedded in the concept of system design is the idea of co-optimization that refers to the simultaneous optimization of multiple interconnected systems or components to achieve a global optimum that benefits the entire system. Consideration of interactions and dependencies results in an enhanced overall performance. In addition to offline optimization, online optimization is also required in digital twin design. Such optimization is required when the twin has been deployed and is in use. Examples of this include manufacturing process planning or critical vehicle path determination under changing operating conditions.

3.1 Offline Optimization: Offline optimization is performed in several key areas of digital twin design to ensure their effectiveness and efficiency. Prime examples of these areas include model calibration, optimal instrumentation of the physical asset, process optimization including sub-system integration, and scenario analysis and planning among others. A few of these problems are examined next with a view of looking at special aspects of the optimization problem.

3.1.1 Parameter Calibration: Approximating the behavior of physical assets by analytical or numerical models (physics-based, data based) necessitates the selection of model parameters whether they be elements of a physics-based model or parameters of a neural network. Model calibration and model validation are two essential steps in the development and deployment of predictive models. First, it is important to calibrate the uncertain model parameters. While Bayesian calibration methods [106] have been suggested for this purpose and shown to be accurate and robust, their actual implementation is both involved and computationally intense.

Optimization methods provide an alternative approach for this purpose. In this approach a given metric may be maximized or minimized to estimate the problem parameters. The least squares method minimizes the squared error between the known output and that obtained from a predictive model with the unknown parameters. Applications of this approach are presented in [107,108]. Such an optimization-based approach typically produces deterministic estimates of the optimized problem parameters. Use of techniques such as the Markov Chain Monte Carlo (MCMC) [109] has been proposed to mitigate this drawback. To do this one assumes a prior distribution for the parameters to reflect initial uncertainty. One also defines a likelihood function based on observed data and then combine the priors and likelihood using Bayes' theorem to obtain the posterior distribution. The MCMC algorithm is used to sample from this posterior distribution, generating a range of plausible values for the parameters allowing for uncertainty quantification in model predictions.

The choice of the optimization algorithm itself is problem dependent, ranging from linear least squares approach to gradient based nonlinear programming algorithms, and metaheuristic random search algorithms such as genetic algorithms and simulated annealing.

3.1.2 Instrumenting the Physical Asset: Another offline optimization application is the optimal instrumentation of the physical asset to maximize the effectiveness of the digital twin. An example of this is to determine the optimal number of sensors (of different types) and their location on the physical system. This has a bearing on both the volume of data and its accuracy and would impact the eventual usefulness of the digital twin. Competing criteria such as power requirements, cost, robustness of system under partial degradation, etc., are in play, and this makes for a challenging multicriteria optimization problem [110,111]. The formulation of the optimization problem – how the objective criteria are defined, the choice of design variables, and constraint formulation present interesting and challenging optimization problems.

Broadly speaking, this is a topology optimization problem that lends itself quite well to heuristic search algorithms such as genetic algorithms. Applications using this approach [112,113] have been proposed, including cases where the problem is formulated as a multicriteria design problem. This problem is also one where it is important to consider aleatoric uncertainty in the design process. Given that there is natural variability in sensor quality, it is important to include this effect in the optimal design process.

The choice of the objective function for optimization, formulating the uncertaintybased optimization, and using appropriate technique to perform this optimization represent the principal challenge in this problem. The most used objective criteria include *probability of detection* that minimizes the number of false positives and negatives [114], the *information gain* criterion that uses quantitative metrics to measure the usefulness of data collected in a sensor network [115,116], and the *value of information* criteria that measures the value of data collected from a particular location by comparing that location against others in the domain [117]. A combination of these criteria can be used in the optimization process by interchanging criteria with constraints.

Once a model has been calibrated, it must still undergo the process of validation which confirms that the model of the physical entity conforms to the expected system performance requirements. The model must first satisfy the face validity test which is largely subjective. Animation and Turing tests have been implemented in this context where the goal is largely one of checking the model's realism when compared against the physical entity. A second, more quantitative test is to compare the actual simulated data against data from the real system and use statistical measures to assess the similarity.

3.2 Online Optimization

Once the digital twins have been developed and deployed, their operation calls for the continual use of optimization techniques for getting the most out of their availability – the capability to simulate, predict, and optimize performance enables more informed decision making. This online optimization must provide real-time performance and special approaches have been developed to accommodate this requirement. Real-time performance is defined [99] as *"…the minimum computational speed required to achieve seamless and uninterrupted optimization, prediction, and control of the system of interest."* In real-time optimization, the optimized design set is re-computed on a regular basis. – these could vary significantly depending on whether the digital twin is assisting with operational control, providing insight into an allocation problem, or assisting with scheduling such as preventative maintenance. A hierarchy of process control activities adapted from [118] is shown in Figure 11. It is not always easy to ensure that sensing, prediction, and control can be performed at the desired time scales and approximations are necessary to get the desired feedback; such feedback must be accompanied by statistical levels of confidence.

Figure 11: Hierarchy of Process Control Activities

Examples of such hierarchy have been cited in the literature [119]. A digital twin designed for electric car battery management system could afford an online optimization that may take several hours or even days because of the relatively long operational life of the battery. On the other hand, a digital twin designed for structural health monitoring may require optimal feedback from the system at time scales of the order of micro-seconds [120]. Some of the available approaches for such applications are described in subsequent sections.

3.2.1 Real-Time Optimization in Manufacturing: Reinforcement learning (RL) has been used to optimize a digital twin for a manufacturing process (plastic injection molding) [121]. The flow of information between the physical and digital entities is shown in Figure 12. The process of training and deployment requires an environment to be defined that includes the state of the system (e.g. status of parameters like temperature, speed, pressure, energy consumption, and defect rate). An action space which refers to adjustment to state parameters and a reward function that, for e.g., looks at the combined merit production output, defect rate, and energy consumption. A suitable RL algorithm is deployed to handle the continuous action space. The RL agent consists of a policy network (actor) to determine actions and a value network (critic) to evaluate action quality, is then implemented. The RL agent then adjusts parameters, receives feedback in the form of rewards, and learns to optimize the settings over a period of time. Once trained, the performance of the network is evaluated to assess its generalization capability for previously unseen inputs, with potential fine-tuning of the reward function and hyperparameters to achieve optimal results.

Figure 12. Schematic of Online Optimization of Digital Twin (from [121])

3.2.2 Digital Twin for Path Planning: The digital twin offers a continual flow of information between the physical and the digital entities. This allows for the generation of data-driven optimal strategies for path planning in complex situations. Optimized path planning is a critical requirement in areas of logistics, transportation, and manufacturing. By leveraging real-time data and advanced simulations, digital twins enable dynamic and optimized path planning. Virtual models integrate information from sensors, historical data, and predictive analytics to provide a comprehensive and up-to-date representation of the physical environment, allowing continuous monitoring and adjustment of routes based on changing conditions, such as traffic congestion, weather changes, and operational constraints.

To provide real-time optimal path planning that handle dynamic and sometimes uncertain environments, specialized approaches have been developed that are applicable to digital twin usage. A-Star [122] is a popular real-time pathfinding and graph traversal algorithm. It efficiently finds the shortest path from a start node to a target node by using heuristics to prioritize paths that are likely to lead to the goal quickly. Another approach for this purpose is the Dijkstra's algorithm [123], a classic method for finding the shortest path between nodes in a graph. While designed primarily for static environments it can be adapted for real-time applications with frequent updates.

An example of path planning is available in [124] where a high-fidelity digital model of an autonomous ground vehicle was developed that allowed for the prediction of vehicle mobility with changing terrains. It included a probabilistic mobility map which identified permissible and restricted zones for the vehicle. Bayesian model updating schemes were used to update the model which then allowed for real-time mission planning. RL algorithms, such as Q-learning and Deep Q-Networks (DQN), learn optimal policies by interacting with the environment and receiving rewards or penalties. They have been applied for real-time path planning [125] as they allow for continuous learning and adapting to new conditions. It should be mentioned, however, that RL based methods require significant amounts of data and may be quite challenging to implement in practical applications. The nature of the optimization problem, most critically the definition of the objective criteria, has a significant influence on the methodology used in practice.

3.2.3 Co-optimization and Digital Twins: Co-optimization refers to the simultaneous optimization of multiple interrelated systems or processes to achieve the best overall performance or outcomes. It has been stipulated earlier in the paper that digital twins are indeed representative of the framework of a *system-of-systems*. In this context, therefore, co-optimization facilitates the design of such a system by allowing for the inclusion of both performance characteristics and operational efficiency through the entire life cycle. By integrating real-time data from physical assets with advanced analytics, digital twins facilitate improved designs with superior decision-making and resource allocation. For example, in smart manufacturing, cooptimization can help balance production schedules with energy consumption, leading to significant cost savings and reduced environmental impact (126). This approach enables a holistic view of systems, allowing for adaptive strategies that respond to changing conditions. A challenge in this work is in the creation of appropriate merit functions that include not only traditional design variables but also policy functions that control operations. These ideas are discussed in [99] in some detail.

The challenge in implementing this approach is multifaceted – establishing a hierarchical breakdown of the problem domain (system decomposition), creating component/subsystem response approximations with the fewest number of state variables that capture the essence of the behavioral response, quantifying the uncertainty in these approximations, and selecting the optimization framework and the underlying optimization algorithms that best manage the coupling within and among the subsystems.

In addition to formal methods of decomposition described earlier, domain knowledge and user experience helps define the initial decomposition topology of the problem structure. Simultaneous execution of low fidelity models of the components/subsystem helps understand how changes in one part of the system affect the outcome of others. After this step, an integrated modeling and simulation strategy is adopted which allows model refinement over several time steps. This is schematically shown in Figure 13 that has been adapted from [127].

Figure 13. Optimizing Physical and Digital Assets Over Time

This refinement is based on the use of real-time data from sensors and IoT devices, and robust strategies for integrating this data across all relevant subsystems are required to enable dynamic adjustments and continuous improvement. Continuous monitoring and adjustments are made based on real-time feedback and evolving conditions to ensure that the system remains optimized even as external factors change. Advanced optimization strategies and machine learning algorithms are foundation for co-optimization. These tools assist in not only parsing vast amounts of data to identify emerging patterns but also are an aid in the solution of the nondeterministic optimization problem. The formulation of the optimization problem has its own challenges, in particular formulating merit or reward functions and constraints for problem.

4 AR/VR Integration in Digital Twins

The integration of augmented and virtual reality (AR & VR) technologies in digital twins offers transformative possibilities across different applications [128]. While these efforts are mostly at a speculative stage or in early stages of development, they are targeted to developing features in the digital twin platform that would allow users to visualize and interact with these digital replicas in immersive and intuitive ways. The focus thus far has been on production processes, service design, and Human– Machine Interaction. AR overlays digital information onto the real world, allowing users to see and interact with a digital twin in its actual physical context. As an example, manufacturing workers performing maintenance can use AR glasses to visualize the inner workings of machinery, providing step-by-step instructions directly in their field of view. VR on the other hand provides a fully immersive experience where users can interact with a digital twin in a simulated environment. This is particularly useful for training and simulation, enabling users to practice complex procedures without the risk associated with real-world operations.

Among the most often cited potential applications of AR/VR in this application is in maintenance and repair operations. Real-time sensor data available to the digital twin can identify emerging maintenance needs or imminent failure. VR can be used to practice a repair procedure on the digital model before performing it on the physical asset. Engineers and designers can also use AR/VR to interact with digital twins of products during the development phase. Geographically dispersed teams can come together in a shared virtual space where they can interact with the digital twin in realtime. This feature also has merit in performing design reviews, as dispersed stakeholders can experience and evaluate the product in a virtual space, identifying potential issues and improvements before physical prototypes are built.

GE Healthcare has used AR with digital twins of their medical devices to provide realtime support and training to technicians, ensuring efficient maintenance and operation. Similarly, Volvo Group has used AR technology to reduce time and costs associated with the quality assurance process in their engine assembly facility. Another noteworthy application has been in the creation of the digital twin of an entire production factory by BMW. Engineers at BMW and NVIDIA deployed VR to create these digital twins [129] with the specific target of optimizing workflows and ergonomics before physical changes are implemented, saving time and resources.

The impact of extended reality tools in a digital twin environment is explored in [130]. This is an emerging field of research, and many technical challenges persist arising from the need to integrate complex systems, ensure real-time performance, and provide a seamless user experience. AR/VR hardware must continue to evolve and become powerful enough to handle complex computations. Existing hardware limitations can restrict the performance and usability of AR/VR in digital twins [131]. It is important to ensure that AR/VR systems and digital twins work seamlessly with other technologies and platforms; this requires interoperability standards and protocols to be developed and adopted [132]. Additional challenges in this field include the following.

- (i) Data integration and management is critical in digital twins and integrating this data into AR/VR environments in real-time is a significant challenge.
- (ii) Real-time processing is important for an immersive AR/VR experience. Achieving low latency in data transmission and processing is critical [133].
- (iii) AR/VR applications require high-quality graphics and rendering to provide realistic and immersive experiences. This demands significant computational

power and advanced rendering techniques, which can be resource-intensive [134].

- (iv) The design of intuitive and effective user interfaces for AR/VR environments is complex. Users must be able to interact with digital twins naturally and efficiently, which requires innovative UI/UX design and human-computer interaction techniques [135].
- (v) The ability to scale AR/VR applications for digital twins to complex environments with multiple users can be challenging. Ensuring consistent performance and quality across different scales requires robust and flexible system architectures [136].

5 Closing Remarks

The paper has focused on the field of digital twins as a rapidly evolving discipline within the realm of digital technology and data analytics, and that has an important emerging role in transforming many application domains by making available a powerful tool for simulation, analysis and optimization. The digital twin is a virtual representation of a physical object, system, or process. It differs from the tried and tested simulation model due to the continuing use of real-time data and historical evidence to enable learning, reasoning, and dynamically recalibrating for improved decision making.

The paper posits that viewing digital twins as a system of systems allows for a more comprehensive and integrated approach to design such a system. This perspective provides for an opportunity to adapt various developments from the field of multidisciplinary design optimization (MDO) in this problem. Using formal methods of system decomposition to reduce the optimization of a complex system to smaller coupled subsystems is noted as a natural first step. In addition to establishing a topology for decomposition, tools developed to ease the computational burden of repetitive function analysis for optimization are directly applicable in this domain. Methods for function approximation including polynomial response surfaces, Kriging, machine learning based approximation, as well as hybrid approximation that combine the relative merits of physics-based and data-based models, are all applicable in the digital twin design and deployment. Methods to account for uncertainty quantification in such modeling, are also important in this context given the significant simplification that is often required for modeling very large and complex coupled systems. Similarly, MDO spurred developments in optimization methods for high dimensionality design problems are also adaptable to this problem domain, including considerable work done around optimizing in the presence of uncertainties.

The paper identifies areas for continuing research and development. Continued and meaningful use of digital twins will require new advanced real-time analytics and predictive modeling capabilities. Using real-time data and processing this data at the edge in a low computational resource environment should be the motivation for such efforts. Additionally, the task of data management and data integration becomes critical in this environment. Research needs to be directed at developing robust data integration frameworks that enable real-time data processing, storage, and retrieval while ensuring data quality and consistency. Interoperable systems and standardized protocols represent another area of research focus. The lack of common standards hinders seamless integration and communication between different digital twins and their corresponding physical counterparts. Universal standards that ensure compatibility across various platforms and technologies need to be developed and implemented.

There is a need for developing intuitive interfaces and visualization tools that enable users to interact seamlessly with Digital Twins. Advances in AR/VR and their potential to drive new innovations in digital twin implementation have been discussed. Continuing research is needed to develop innovative ways to present complex data and insights in a user-friendly manner, enhancing decision-making processes. Even as these advances materialize, one cannot ignore the importance of cyber threats in such systems – the vastly interconnected digital and physical systems provide greater exposure to data breaches, and research in developing robust defense mechanisms for such architectures must be explored.

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