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On the Formalization of Development and Assessment Process for Digital Twins

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INTRODUCTION

In recent years, autonomous control systems have been encouraged in advanced reactors to help restore economic viability, simplify operations and maintenance, and enable remote-site power generation [1]. Because the reactor is expected to operate for a long period with a limited individuals onsite, it is recommended that the autonomous control system have access to very realistic models of the state of processes throughout the lifecycle, together with these process behaviors in interaction with their environment in the real world. As a result, digital-twin (DT) technology is suggested in autonomous control systems. DT is defined as a digital representation of a physical object or system that contains a record for the histories of loads, operations, and maintenance status, predictions for the near-term transient of important state variables, and decision-making processes [2].

Because machine learning (ML) can recognize patterns within a complex system in real-time applications, it has been used to build DTs in autonomous control systems for advanced reactors. Meanwhile, due to the rarity of operations data in accident scenarios, the development and assessment of DTs is expected to be mainly driven by simulations. Although the capability and feasibility of ML-based DTs are recognized to improve safety and efficiency of reactor control, a major concern from the regulatory commission and the nuclear industry is whether the information from a DT is developed and assessed in accordance with expectation and requirements by the target decision. These concerns not only affect the acceptance criteria for DTs, but also values that can be extracted from DTs and autonomous control system during operations.

Inspired by the success of formal methods of improving the reliability and robustness of computer programming and software development, it is suggested that the development and assessment process (DAP) for both separate DTs and integral control systems should be formalized in a transparent, consistent, and improvable manner. In this study, a digital-twin development and assessment process (DT-DAP) is proposed by adapting the evaluation model development and assessment process (EMDAP) [3] to requirements of the autonomous control system, ML algorithms, and DT technology. To demonstrate the framework, a baseline nearly autonomous management and control (NAMAC) system, with ML-based DTs for diagnosis and prognosis, is developed and assessed based on the framework. It is found that, with selected testing methods and techniques, the DT-DAP can help identify errors in DTs and NAMAC that would otherwise be left unverified. Meanwhile, it is found that the DT-DAP can improve the DTs and NAMAC by continuously learning and iterating through different elements.

DEVELOPMENT AND ASSESSMENT PROCESS FOR DIGITAL TWINS IN AUTONOMOUS CONTROL SYSTEM

A DT shares many commonalities with modeling and simulation (M&S): both a DT and M&S are designed to virtually represent the behaviors of physical systems [4]. However, M&Ss are applied mainly in the phase of system design and developments—e.g., to support design takes, to validate system properties, or to provide a better understanding of physics—and they have rarely been integrated with real-time and continuous management of physical systems during their lifecycles [5]. As for DTs in the autonomous control system, they are developed as digital representations of physical objects or systems. To be specific, a DT can be used to read real-time and past-history data for inferring complete reactor states, finding available control actions, predicting future transients, and identifying the most-preferred actions. During the operation of a nuclear power plant (NPP), DTs can help decision-makers sustain an accurate understanding of the physical system, improve the effectiveness of control, and avoid human errors in decision-making. Therefore, the DT-DAP is required to merge knowledge base and real-world information in all life-cycle phases and to optimize operations and controls based on real-time simulation-based solutions.

ML includes a variety of methods: neural networks, support vector machine, decision tree, etc. ML has shown great success in regression, pattern recognition, and image processing [6]. An artificial neural network, as an example, is a model of computation inspired by the structure of neural networks in the brain. In this simplified brain model, a neural network is defined by "a large number of basic computing devices (neurons) that are connected to each other in a complex communication network, through which the brain is able to carry out highly complex computations [7]." In recent research, it was proved that a network with two layers and suitable activation function can approximate any continuous function on a compact domain to any desired accuracy [7]. However, to have the best approximation to a limited set of data, a large number of hyperparameters need to be tuned. According to the no-free-lunch theory, there is no network structure, training scheme, or set of hyperparameters that is universally better than any other. The best algorithm has the same average performance as merely predicting that every point belongs to the same class [6]. As a result, the DAP for ML-based DTs should evaluate uncertainty from a high-dimensional parameter space. Meanwhile, it should actively adapt to changes in environments and applications by updating network structures, training schemes, and hyperparameters based on the evaluated uncertainty.

The EMDAP [3] is a framework that integrates requirements, knowledge-based generation, model development, and assessment throughout the M&S life cycle. Developed by the U.S. Nuclear Regulatory Commission, EMDAP aims to describe an acceptable process of developing and assessing the evaluation models that are used to analyze transient and accident behaviors within the design basis of an NPP. Figure 1 adapts the EMDAP to the DT-DAP. The development and assessment of DTs are performed by training and evaluating an ML model based on the requirements and knowledge base. Element 1 aims to establish requirements for the DT, including the purpose of the control system, transient class, DT's interface, model, and function, reactor types, etc. Based on the requirements, Element 2 aims to construct a knowledge base that includes the issue space, simulation tool, and data repository. The issue space defines the scenario in mathematical formulations. The simulation tool (system code with adequate fidelity) is required to generate the training/testing data set for the development of different DTs. The data repository has two elements: the knowledge element and the data element. The knowledge element consists of literature or information related to operating procedures and training materials, system configuration, initial conditions, reactor failure modes, experimental data, benchmarking results, etc. The data element consists of data generated by the simulation tool for the development of DTs and to plant data collected from operational histories, transients, and events. Next, Element 3 develop DTs based on the knowledge base by Element 2 and requirements by Element 1. For ML-base DTs, Element 3 establishes a training plan, including the training scheme, sets of hyperparameters, input/output features, normalization techniques, etc. Next, based on the knowledge base, the DTs are assessed in two parts: bottom-up approach and top-down approach. The bottom-up approach evaluates the performance of separate DTs, including their performance, generalization capability, and fidelity to proper subsets of the knowledge base. The top-down approach is to evaluate the overall performance of NAMAC with implemented ML models as DTs, including their applicability to the control system, DTs interactions, and the performance and generalization capability of the autonomous control system. Finally, Element 5 decides the adequacy of DTs and autonomous control system based on the requirements, knowledge base, DT implementation, and DT assessment results. If DTs and the corresponding system are adequate, they are applied to target reactors, transients, and scenarios for risk analysis. If DTs and NAMAC do not meet the adequacy standard, users need to return to appropriate elements for corrections. The iteration will continue until all adequacy standards are met.

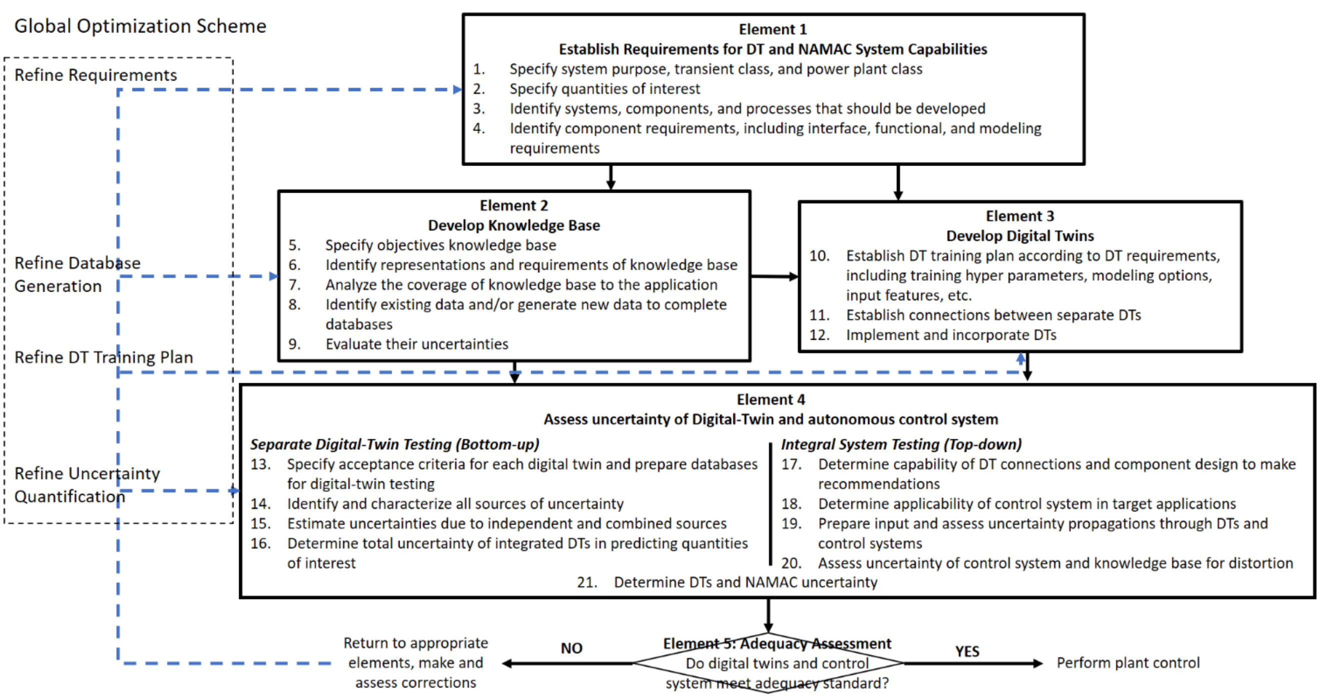

Figure 1: Scheme for the DT-DAP. Adopted from EMDAP framework [3]

Considering the complexity of the reactor system and the development process, the DT-DAP is classified into two phases: scoping and refinement. In all phases, it is required that DT prototypes and instances are implemented in the designed environments for the target applications. Meanwhile, it is also required that DT errors be analyzed and that they satisfy the acceptance criteria. At the scoping stage, the DAP is mainly driven by expert knowledge and user experiences while assessment techniques are largely qualitative, including both sensitivity and uncertainty analysis. The goal is to identify sources of uncertainty, evaluate their relative importance, and optimize the training plan based on experiences. However, there are potentially large uncertainty and bias due to the limited knowledge of user groups. Although the DT performance satisfies the acceptance criteria, it could be only applicable in the training domain or a specific class of scenarios. As a result, when the DTs and control system are applied to different transients, their uncertainty can be so large that it could alter other DTs and final decisions. In such conditions, the trustworthiness of the DT and control system needs to be carefully investigated.

At the refinement stage, the major sources of uncertainty and bias are refined by improving users' knowledge or by formalizing the DAP with mathematical languages. The DT uncertainty can still be large; however, they should be better characterized and continuously decreased in a consistent and transparent manner. Uncertainty quantification is one of the major techniques in the refinement stage that refers to the activity of identifying, understanding, and quantifying all possible uncertainties within the system of interest [8]. For ML algorithms, Bayesian inference can be used to optimize hyperparameters based on a prior distribution and additional observations [9]. Interval analysis is used to accelerate the convergence of ML to the global minimal point or to guarantee that all solutions are found to any degree of accuracy with guaranteed bounds [10]. Meta-learning, i.e. learning to learn, divides a large learning task into two hierarchies of learning: base learner and meta learner. Compared to the classical training for ML-based DTs, denoted as the base learner, there is also a meta model that optimizes the base learner by updating its parameters via a meta-knowledge base [11]. In addition to the separate DTs development and assessment, the quantitative software-reliability method evaluates the reliability of the autonomous control system by quantifying the software failure rates and demand-failure probabilities of digital systems in NPPs. As a result, at the refinement stage, the impacts of uncertainty and bias on operators' decisions and directly connected DTs are known, and resources can be directed to areas with insufficient knowledge. A formalized framework for knowledge elicitation or parameter optimizations is required to improve efficiency and effectiveness in resource allocations.

At the maturation stage, DTs and the autonomous control system become mature, where uncertainty and bias are minimized with the currently available methods and techniques. To demonstrate the use of DT-DAP, a baseline NAMAC system is developed with four DTs at the scoping stage, where the DT for diagnosis (DT-D) and the DT for prognosis (DT-P) are implemented with ML algorithms.

DEVELOPMENT OF A NEARLY AUTONOMOUS MANAGEMENT AND CONTROL SYSTEM

A NAMAC system is designed to provide recommendations to the operator for maintaining the safety and performance of the reactor. The NAMAC system utilizes simulation-informed, data/knowledge-driven, AI-guided, plant-data-assimilated real-time operating procedures to effectively support the operator in all operation modes. Besides relying on operator's knowledge and judgment, NAMAC is designed to furnish recommendations to operators for effective actions that will achieve particular goals, based on the NAMAC's knowledge of the current plant state and prediction of future state transients while reflecting uncertainties that complicate the determination of mitigating strategies. Knowledge is extracted from the knowledge base and stored in DTs of various functions. There are four key DTs while the diagnosis and prognosis DTs are developed with ML algorithms. The objective of ML-based DT-D is to construct a relationship between correlated state variables based on the knowledge base. In NAMAC, DT-D is used to determine the unobservable safety-significant factors, including peak fuel centerline temperature and peak cladding temperature, based on observed sensor data. The DT-P aims to predict the future transients of state variables or lifecycles of certain components based on past histories and current information. In NAMAC, a DT-P model is trained to predict the consequence factor of control actions based on reactor information at the recommendation time point.

DTs are connected based on an operational workflow as the autonomous control system. The DT-D reads sensor data from the reactor or simulator to monitor unobservable state variables, and the objective is to restore complete information about the reactor. The obtained values are fed to (1) DT-P for predicting future transients (2) strategy-inventory DT for determining available control actions (3) discrepancy checker for continuous monitoring. The DT-P reads reactor information from DT-D, together with available control actions, to predict the future transients of reactor states or consequences over a certain time range. The DT-P outputs are mainly used for deciding the best strategies according to certain preference structures that represent the preference of the operator or risk-management team to the economic and safety of a reactor.

Guided by the DT-DAP, DT-D and DT-P are implemented with ML algorithms—i.e. feedforward neural nets— and assessed as separate DTs and within the NAMAC system. Requirements (Element 1) are set up based on the NAMAC objective and operational workflow. Meanwhile, Experimental Breeder Reactor-II (EBR-II) and a partial loss of flow accident (LOFA) due to primary sodium pump (PSP) malfunctions are selected as the type of reactor and transient respectively. A knowledge base (Element 2) is constructed by first characterizing the LOFA issue space based on the speed curves of two PSPs. Next, a GOTHIC model for the primary side of EBR-II is constructed and benchmarked against experimental data [12]. A data repository is built by coupling GOTHIC with a statistical software named RAVEN for sampling, data generation, and storage. To train ML algorithms for DT-D and DT-P (Element 3), the database is first separated into training and testing according to the issue-space characterizations. To test the generalization capability of DTs, the testing data contains "unseen" data points outside the training domain. Driven by user knowledge and experience in ML training and testing, the ML-based DT-D is developed, and its training root mean square errors equal 1.42℃ and 0.54℃ respectively. To assess the performance of DTs, they are first evaluated separately. It is found the L1 relative error norms of both DT-D and DT-P in the testing domain are less than 5%. Other sources of uncertainty, including input time ranges, sensor failures, and target training losses, are evaluated and found to be strongly correlated with the error of DTs. Next, these DTs are assembled into NAMAC, and the NAMAC is further tested by coupling it with the GOTHIC plant simulator. A confusion matrix [13] is defined to visualize and quantify the accuracy of the NAMAC system in classifying the predicted consequence of control actions. It is found, when NAMAC is operated within the training issue space, the confusion ratio equals zero, indicating a reasonable recommendation that is consistent with the historical norm of human operation. However, when the issue space is outside the training domain, the confusion ratio grows, indicating the recommendations are either too conservative or could lead to component failure. More details regarding the ML algorithms, training, testing, NAMAC assessment, etc. can be found in [14].

RESULTS

To improve the reliability and robustness of DTs and the corresponding autonomous control system, a DT-DAP is developed for both separate DTs and integral control system. The framework is designed by adapting the EMDAP to requirements of the autonomous control system, ML algorithms, and DT technology. To demonstrate the framework, a baseline NAMAC system with ML-based DTs for diagnosis and prognosis are developed and assessed based on the framework. It is found that, with selected testing methods and techniques, the DT-DAP can help eliminate major sources of uncertainty in DTs that impact errors of DT and NAMAC. Meanwhile, it is found that DT-DAP can improve the quality of DTs and NAMAC by learning from explicitly documented elements and procedures. At last, it is recommended that quantitative and self-learning algorithms should be adopted to further refine and accelerate the development of DTs and NAMAC.

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