

THREE CARRIAGES DRIVING THE DEVELOPMENT OF INTELLIGENT DIGITAL TWINS – SIMULATION PLUS OPTIMIZATION AND LEARNING

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ABSTRACT

Three key technologies are driving the development of intelligent decisions in the era of Industry 4.0. These technologies are machine learning, optimization, and simulation. It shows that solely relying on one technology is not able to meet the decision timeliness and accuracy requirement when solving current industry decision problems. Thus, to meet this challenge, this paper firstly discusses several possible integrations among the three technologies, in which simulation plays an important role in depicting the system models, generating data for optimization and learning, and validating optimized decisions and learned rules. A number of future research directions are pointed out based on the gap between the current technology / tools development and the industry needs. Finally, the paper proposes a possible collaboration mode among higher learning institutes, research institutes, equipment and platform developers, as well as end-users for better shaping the whole intelligent decision ecosystem.

1 INTRODUCTION

In the past few years, the human industry evolution is gradually marching on to the era of Industry 4.0. From the angels of data and computer-aided decision, there are three key technologies emerging and are shaping the future of every industry.

First of all, a huge amount of data has been accumulated along with the development of internet, which brings about data science and machine learning. Industry players put more and more attention on the value of data in those customer-driven industries, such as the retailer and service industries. Nowadays, a common sense is gradually emerged: data is the king. Data analyst is also becoming a popular occupation in great demand. As an advance tool, machine learning tends to become the first choice in data analysis, replacing the classical statistics method. The trend is spreading rapidly to other industries, such as transportation and manufacturing industries.

On the other hand, although optimization technology has been developed to an extent, the recognition and usage of which in the real-world applications is still limited. It has to admit that in most of the traditional industries, industry players tend to rely more on their past working experience when making decisions; the output from optimization algorithms is used only as the reference to the decisions considering assumptions. Moreover, the efficiency of solvers has also limited the usage of the technology. The situation has not enhanced much even if the performance of computing and solver has been improved, which carves out a promising research direction for many generations of researchers.

Simulation seems to stand alone in the technology expressway, maintaining a lukewarm relationship with the other two carriages. It seems that the application of learning and optimization is not affected without adopting simulation. Thus, researchers tend to see simulation as “the icing on the cake”, or a makeshift technology before other technologies are completely ready, instead of a core technology in the ear of Industry 4.0. Moreover, researchers and industry players have different views when talking about simulation. Even within industry, different sectors would have different definitions of simulation, thus the popularity of simulation is various among sectors.

A common sense is gradually shaping in both of the academia and industry that to solely rely on one technology when solving real industry problems is insufficient in the ear of Industry 4.0. Thus, this paper analysis the possible interaction among the three key technologies and proposed a “tech troika” - smart digital twin ecosystem, which integrates the three key technologies in the operational research field. It also proposes a unique view to see simulation as the core technology that buoys up the foundation of the ecosystem. Finally, the buzzword of “smart digital twin” ecosystem could be finally achieved, driving the smart decisions in future economy activities.

2 BACKGROUND

Before any further discussion, it is necessary to review the definition, functions, as well as pros and cons of the three technologies. It is noteworthy that each of the technology has its own subcategorization, and the subcategories may overlap with each other. We will only focus on the unique subcategories; the overlap ones will be focused on in the following sections.

When talking about machine learning, we usually indicate supervised learning, unsupervised learning, and reinforcement learning. Among these types, supervised and unsupervised learning are able to learn rules from the past data and thus to predict for the future scenarios or test on new input data. Reinforcement learning is more powerful than the former two types in terms of its additional ability to dynamically deduct the system status changes and thus guide decision-making. Due to this reason, reinforcement learning could be seen as an initial stage of the combination of simulation, optimization and learning. Thus, it will be discussed in the next section. One of the pros of machine learning is that it could summarize rules of a system without knowing the detailed mechanism of a system, so that the trained model could react fast to the new input. This feature of machine learning makes it ideal for real-time decision making. It must admit that there exist some limitations in machine learning, such as the long training time for more complex model, and the need for a minimum amount of historical data, etc. If solely utilize leaning without simulation and optimization, learning itself could at most avoid some obvious wrong decisions, however, it is unlikely to output the optimized decisions that has never happened in past scenarios. Especially when we face entirely new scenarios or complex systems, the quality of decision generated from learning is quite limited by the short of data volume and poor data quality.

Thus, the importance of optimization is emerged in decision-make processes. The optimized and nearly optimized solution could be obtained from algorithms if elements in a system and interactions among those elements are able to be clearly described. These elements include, parameters, decision variables, constraints, and objectives. Comparing to learning, optimization doesn't need to rely on huge amount of historical data and is possible to output results that are superior to any past ones. This pro of optimization is critical in industry decision problems such as new system design and old system modification. Nevertheless, there are cons existing in this technology, showing in the difficulty to tradeoff between model fidelity and computing efficiency. Also, some high-performance algorithms, such as the simplex algorithm, would require the formulation of the problem to be linear. This restriction adds on the difficulties when describing the real industrial systems. Also, because of assumptions made in the model, there is always a gap between the optimized solutions obtained by mathematics models and the real optimized solutions. The compromise is that if the restrictions are not considered, the high computing speed is not able to achieve. Besides, consider the dynamics and randomness attributes in most of the industry systems, to describe the system in high fidelity itself is not an easy job. It needs to admit that the aim of the traditional optimization methods

in both literature and industry is to output a nearly optimal solution within a reasonable period of time, instead of using it to perfectly describe a complex system or to test solutions in real running systems.

Simulation is an ideal technology which could compensate the limitations of the other two technologies mentioned in the previous paragraphs. Simulation is able to model real systems as standard processes. The interaction between entities and events are simulated along with the time so that KPIs could be computed and output. The major purpose for us to establish a simulation model have three folds (1) to depict the real-world dynamics with a certain fidelity level required by the problem statement; (2) to provide a virtual environment which evolve the dynamic systems and evaluate their KPI changes under different input scenarios and decisions; (3) to provide a platform to evaluate the optimization algorithms derived from static and/or simplified models. It has to admit that simulation model itself does not consider how to learn rules or obtain optimal solutions for decisions. Only by integrating simulation with other two technologies could achieve the purpose for decision. Moreover, in most of the cases, modelers are using commercial software due to the complexity in looking into simulator module's black box. The usage of pre-established modules hinders the modelling of complex systems and further adds on difficulties to the integration with the other two technologies.

Overall speaking, the different attributes, purposes of the “three carriages” and the real needs from the industry lead to a promising direction. The most effective combination ways of the three technologies becomes a trend in the current practice and has many cases achieved. In the next section, we will discuss about the combination of optimization and learning first followed by how the combination of the two integrates with simulation.

3 INTEGRATED OPTIMIZATION AND LEARNING

Learning and optimization always go together. In the past literature and applications, the integration of the two are often seen. First of all, how to choose the most appropriate model is in essence an optimization problem, which could be seen as a ranking and selection problem given finite solution space. Secondly, the training of the learning model could be seen as another optimization problem. The objective is to minimize the gap between learning results and the ground truth (if applicable) by adjusting learning parameters or to minimize the training time. For example, the choice of the number of layers and number of features in each layer in a neural network. This type of optimization could be seen as a large-scale search problem. When there exist multiple measurements, the essence of the problem is seen as a multi-objective optimization problem.

We can say that there is a primitive optimization problem in each learning problem. To talk about learning on its own has no meaning if higher accuracy is a requirement. The improvement of the optimization algorithm would enhance the learning efficiency. However, it needs to be clarified that the optimization problem talked here is different from that in a decision-making problem.

In the above two types of integration, optimization is used to support learning. On the contrary, learning could also be used to enhance optimization efficiency. For example, by using partial search results, through learning, it is able to learn the distribution of objective values in the solution space and thus predict the more promising search areas.

An advanced integration of learning and optimization happens in the decision making for dynamic environment. If we see optimized decision as a function of system state under a certain environment, decisions will change along with the changes of environment. Since the change is real-time, no matter how high performance an algorithm is, it is very difficult to achieve real-time optimization, especially for complex systems. An achievable way is to move the optimization offline. It is able to learn the optimized results under various scenarios offline and used the trained model online for decision making. By doing so, the long computing time and fast-computing requirement are decoupled. At the same time, the quality and speed of decision can be guaranteed.

Currently, there are several applications adopting the above type of integration, such as autonomous driving and AlphaGo. For autonomous driving, the offline training identifies the relationship between

environment parameters and driving decisions, and apply them in an online scenario to control the vehicle in real-time. However, most of the data used for the training are generated from the optimized experience of manual driving now. In the real-time decision of AlphaGo, the Monte Carlo tree search serves as the optimizer to provide training data for the deep learning in the entire deep reinforcement learning process. It is noteworthy that although there are many applications under dynamics conditions, this type of integration could also be utilized for the decision-making in discrete-event systems and independent static problems.

As discussed above, one of the major resistances to apply optimization in real time situation is the difficulty in the tradeoff between computing efficiency and decision accuracy. Nowadays, the headache of computing efficiency is almost solved or at least have a direction to solve by offline learning and other emerging technologies. A new research question is asked, can we now have higher requirement on the accuracy of the decision? By doing so, we may need to enhance the fidelity of the model. Only by depicting the real world to the utmost extent can we generate decisions and get them validated with higher accuracy. For example, the success of AlphaGo largely depends on the exact description of the Go rules in the reinforcement learning. So, if we are facing more complex industrial systems, how do we draw the “Go Board”, describe the “Go rule” and depict the interaction between players? To answer these questions, we need to have an in-depth discussion of simulation and is shown in the next section.

4 EXTENSION WITH SIMULATION

From our point of view, there are two major trends that drive a deeper research into the simulation methodologies. One is the integration with optimization and learning, as mentioned earlier. Another trend is the development of automation, which leads to a more detailed and precise control of the equipment and industrial system by computer algorithms. Therefore, the decision-making problems are no longer stay at the planning and designing phase but dive into the engineering details in the system run-time. For example, with the same equipment and layout in a warehouse system, different communication protocols and parameter settings between automated equipment could deeply affect the running performance of the entire system. Considering these factors, a simplified or approximated theoretical model is usually difficult to capture and validate at required details. As a result, there are new requirements raising for the development of simulation methodologies.

In the era of Industry 4.0, firstly (1) simulation shall be capable of precisely describing the detailed state variables of a system and their transitions over time, and therefore, truly reflect the impact of the intelligent algorithms on the system’s performance. Secondly, (2) such details are not necessarily required for analyzing all system problems, considering the computational efficiency. According to a certain hierarchy and based on the problem requirement, the simulation methodologies shall be able to adjust the model fidelity in great flexibility. Lastly, (3) the simulation methodologies shall be friendly to both human and machine interface for reading and writing, form common and practical modeling standards and formalisms, towards various industrial domains. The reason being, in the new application scenarios, the ones who construct and configure the simulation models might be artificial-intelligent algorithms rather than human beings in the future.

Because our focus is mainly on the intelligent decision-making problem in the industrial systems, the type of simulation we are mentioning here is restricted to the discrete-event simulation (DES). It means that in the simulation, we only consider the discrete events happening on the continuous-time horizon and evaluate their impacts on the change of system states. It is well-known and experiments show that, for decision-making analytics, DES is a better way to balance the computational time and evaluation precisions. For DES, conventional modeling approaches include three main modeling formalisms: event-based, state-based, and activity-based (Choi and Kang 2013). According to our past research and practical experience, we conclude the strength and weaknesses of these three modeling formalisms as follows.

Event-based formalism, shown in Figure 1 (a), adopts event-relationship graphs, directly enumerates and describes all the events in the simulation. It has the highest precision to articulate the system’s dynamic transitions. The direct articulation of the system events can effectively connect to the control and decision-

making logic, precisely describe and validate the performance measure of the intelligent systems. However, this modeling formalism lacks systematic and hierarchical structure in handling complex systems and is usually tedious in modeling the details. The formalism is not suitable considering the flexible extension and maintenance of the simulation model. Hence, most of its applications are for theoretical research or education rather than practical applications.

State-based formalism, which is shown in Figure 1 (b), decomposes the entire system into sub-systems as modules in a hierarchical manner according to the structure of state variables, which could also encapsulate the relevant events, and the modules interact with each other via interface events. Because the simulation modules can be configured and reused by just setting parameters, it accelerates the construction and assembly of large-scale simulation models. However, the indirect description of event as internal and external transitions, and duplicated definition of input and output events, cause redundant information, which affects the modeling and execution efficiency of the simulation models.

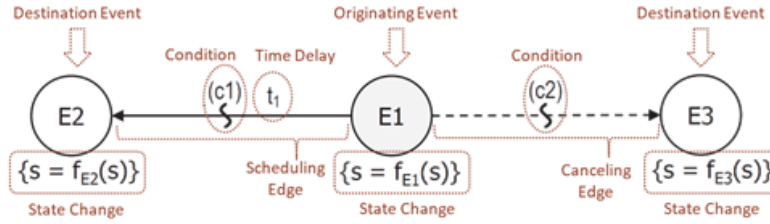
Activity-based formalism, shown in Figure 1 (c), addresses the entity flow in the system, considering the time delay during each activity but not the event at the time point. This approach is intuitive and easy to be understood and operated, thus is used in most commercial simulation software. However, the definition of activity can be rigid and not easy to be extended. In addition, this modeling formalism includes a number of variations, among which, some have ambiguity in the definition of the transition between adjacent activities.

It is obvious that the three DES modeling formalisms meet the requirement of the future development of simulation methodologies from different perspectives, but with respective limitations. Hence, we hope to find a framework, which can be used to synchronize the three formalisms, to keep their advantages, and cover each other on their shortcomings. It is needed to exploit the advantages of simulation on the four different dimensions of a smart digital twin as illustrated in Li et al. (2020), namely (1) visibility, (2) connectivity, (3) fidelity, and (4) analyzability.

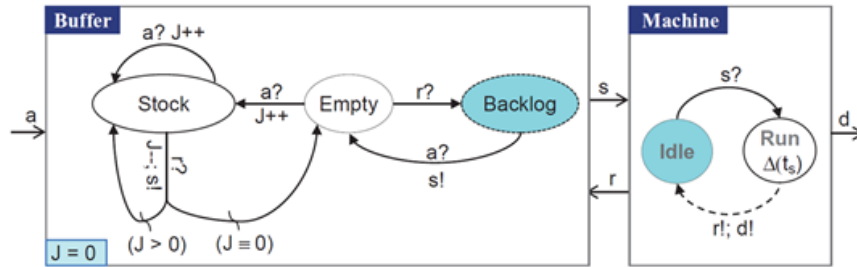
For this purpose, we proposed the O²DES modeling tool in Li et al. (2015). Based on it, we explore such modeling framework. Natively, O²DES is an event-based DES modeling tool, which means, the event-based formalism is the kernel of the framework, and the simulation run is advanced on time by executing the embedded future event list. Because of the advantages of the event-based formalism, we can easily implement the run-time interaction and integration between the simulation and optimization, which includes the optimization-embedded simulation, simulation-based optimization, and parameter tuning in the simulation-based analytics.

Based on it, there is a need to extend such capabilities for the application on more complex industrial systems, such as factories, warehouses, and port terminals, etc. We refer to the state-based formalism and decompose the complex systems into hierarchical sub-system modules according to the structure of state variables. For example, the machine equipment, working units as well as relevant events are encapsulated, encapsulated and finally modeled as various modules, as proposed in Li et al. (2017). In the process of constructing a DES model, the modelers or the artificial algorithms which are responsible for the model building, could simply assemble it by adopting suitable simulation modules which have been prebuilt; the fully understanding of the inner-module details is not necessary. As such, we could consolidate the domain knowledge of industrial sub-systems into the simulation modules, which makes it possible to accumulate knowledge gradually for constructing system models with increasing complexities. In addition, by converting the “open questions” or “essay questions” into “multiple choice questions”, we could enable a better adoption of the intelligent algorithms in the automatic model building process. However, different from a conventional state-based approach, based on the encapsulation with O²DES tools, the event-based kernel is still kept inside the module. As illustrated in Figure 2 (a) and (b), precisely speaking, we are proposing a hybrid formalism, to seek for a balance between the two approaches, and keep their advantages from both sides in the best way.

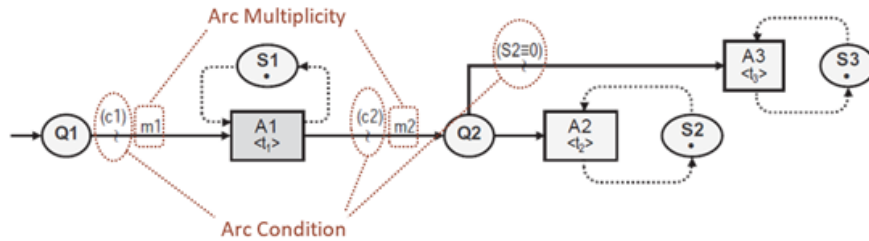
Although the state-based formalism could clearly describe the hierarchical structure of a complex industrial system, it is not flexible in modelling moving materials, for example, the containers in a port



(a) Event-based Formalism (e.g. Event-Graph)



(b) State-based Formalism (e.g. State Diagram)



(c) Activity-based Formalism (e.g. Activity Cycle Diagram)

Figure 1: Demonstration of three DES Formalisms (Choi and Kang 2013).

terminal, and pallets in a warehouse. To achieve such purpose, we need to take the advantage of the activity-based formalism, so that the modelers and/or intelligent algorithms are able to precisely and flexibly master the handling rules of the entity flows. Benefit from the modular development of O²DES tools, we proposed the template of resource-constrained queues (RCQs), as shown in Figure 2 (c), to tackle this issue.

RCQs is an activity-based approach, however, as different from other activity-based tools, RCQs further defines an activity as a special logical module, with common interface events to interact with entities, resources and other activities, including both upstream and downstream adjacent, and activities of other types of entities which need to be synchronized. In other words, although RCQs falls into activity-based formalisms, it is interpreted by the state-based formalism, and executed by the event-based kernel. Therefore, it takes the advantage from all the three formalisms.

The development of the O²DES tool and RCQs template aggregates the three different DES formalism in an organic manner, which effectively supports the development and application of smart digital twins on the four dimensions. As follows, we will briefly elaborate some new opportunities by pointing out the future directions for the theoretical research and engineering development.

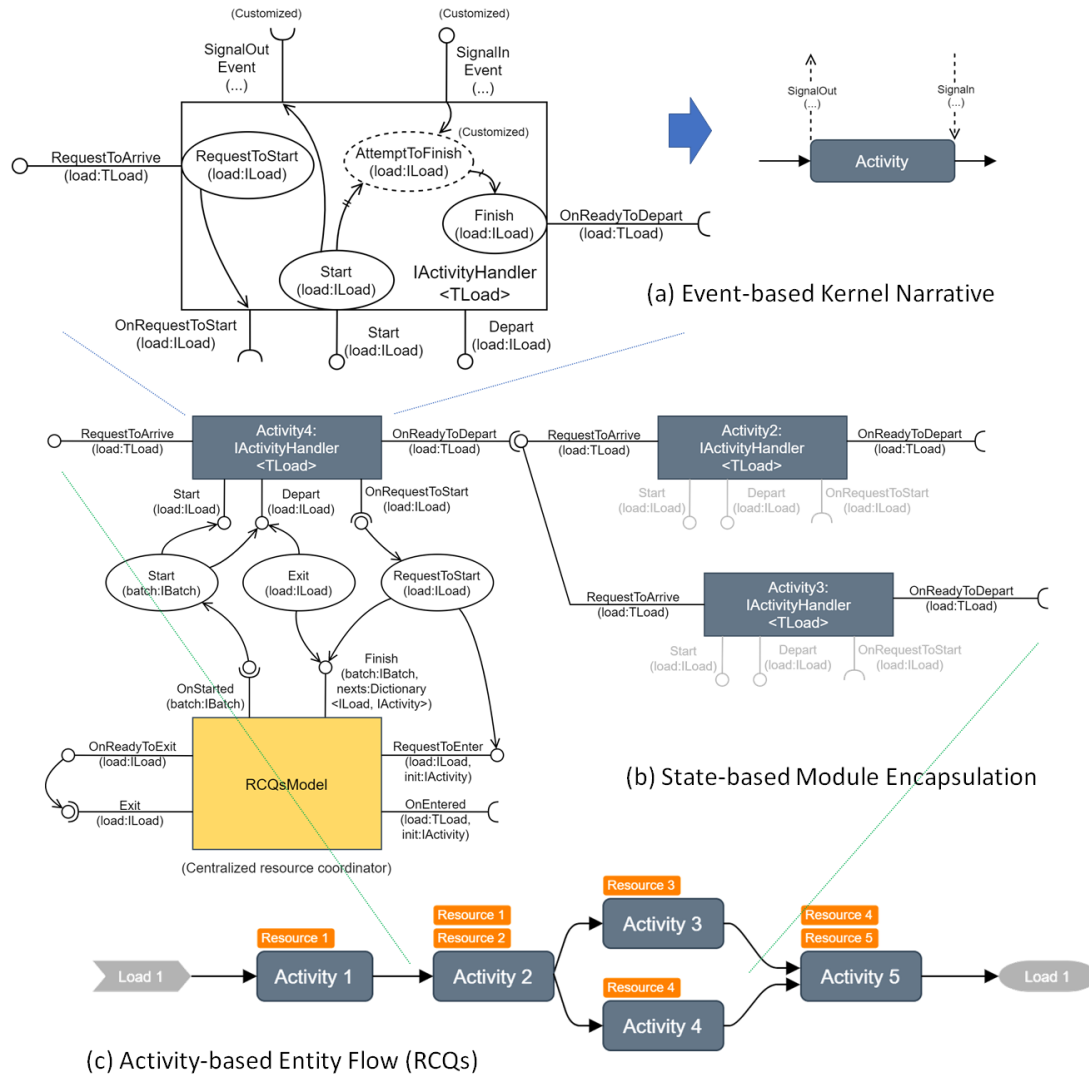


Figure 2: The extended hybrid formalism with O²DES Framework and RCQs.

5 FORMING OF THE THREE CARRIAGES

In this section, we will explore the new directions for the theoretical research from three perspectives of how simulation could be integrated with optimization and learning, including simulation modeling, simulation-based optimization, and simulation-based learning.

5.1 Simulation Modeling

Firstly, from the simulation modelling points of view, although we introduced our practical experience in developing the O²DES tool and RCQs template to realize the aggregation of the three formalisms, it has yet defined an extended formalism on how this shall be done rigorously and scientifically. The continuous research efforts are required to follow the research methodologies of the three existing formalisms. Due to the difficulties in realizing the combination, there calls for a tool that is easy to be used by the modelers. An ideal way is to develop a graphical and algebraic language that formally describes the model in a hybrid manner. It is able to give out suggestions to the choice of formalism and applicable paradigm that fit into various modeling scenarios. By doing so, we shall make the modeling methodologies independent of

specific software tools, so as to provide a general guide for simulation modeling in different development environment. The main research problem shall address how the modeling methodology could efficiently serve the purpose of intelligent decision-making including both optimization and learning. The research on the extended hybrid formalism, could also be further enhanced. The research on the extended hybrid formalism enables modeling researchers to continuously improve the modeling approach, such that it is able to fit industrial application scenarios that are challenging.

5.2 Simulation-based Optimization

From the perspective of optimization, the new modeling formalism could provide higher potential for the development of simulation-based optimization (sim-opt) algorithms. In the past, due the complexity of simulation models, many sim-opt algorithms could only bring in black-box information, i.e., initial input at the start of simulation run, and final output at the end of it. It is extremely difficult to assume any internal mechanism and intermediate information to be exchanged, so that is not able to guide the search algorithms in working in a more efficient manner. With the new formalism, we shall be able to identify certain common structures inside the simulation models with standard performance measures, which can be considered in the design of optimization algorithms. For example, with RCQs template, there can be standard ways to observe the utilization of specific resources and its gradient related information without additional simulation runs; alternatively, we can leverage on the modular hierarchy to dynamically adjust the fidelity of the simulation model adopted in the sim-opt process. Because of the generally defined structure, the simulation model could directly support the calling of such information, and seamlessly applied them into the optimization search algorithms. We could refer to this type of sim-opt as grey-box or white-box optimization. They will enhance the performance of multi-scenario, multi-objective, and multi-fidelity optimization with higher efficiency search algorithms.

5.3 Simulation-based Learning

Other than these, the large amount of data generated from the simulation and optimization process enables machine learning with larger chance to improve the decision-making efficiency and quality. Compared to the pure integration between optimization and learning, the extension with simulation carves a larger room for the aggregation among the three, which can be concluded as the following four types, as shown in Figure 3: (a) to learn the input and output of the simulation, so as to use the learning model to assist or replace the simulation model, for higher efficiency in the simulation evaluation; (b) similar as an intelligent recommendation system, to learn how to rank or select the best among a list of alternative designs, with dynamic and stochastic performance measures; (c) to learn the relationship between changing environment and conditional optimal decisions, so as to response to best action in-time as the environment parameters are keeping changing; and (d) inside a simulation model, to learn the mapping from the sequences of input events and instant state variables to the sequence of output events, so as to simplify the internal structure of simulation models, and ultimately achieve the purpose of automatic digital twining by considering the real physical system with data sensors as the original simulation model.

In addition, in the framework of aggregated simulation, optimization, and learning, we could efficiently control the simulation and optimization process to generate data for higher learning efficiency. This is also a research problem that is worth studying.

5.4 Other Engineering Developments

From the perspective of engineering development, future work could explore the new computational infrastructure, such as parallel computing, cloud-native computing, field-programmable gate array (FPGA), quantum computing, etc. At the same time, to apply such methodologies into industrial practices, we also need to explore the application of IoT and mixed reality to provide rich data to real-time online decision-making and reflect the analytical results to the decision-makers.

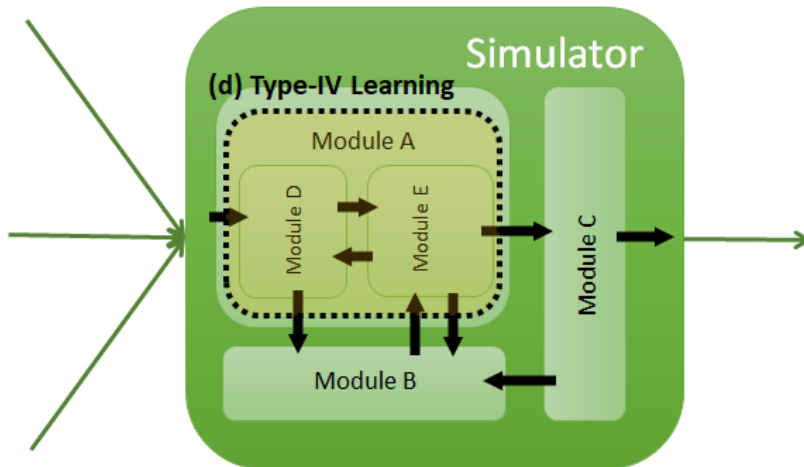
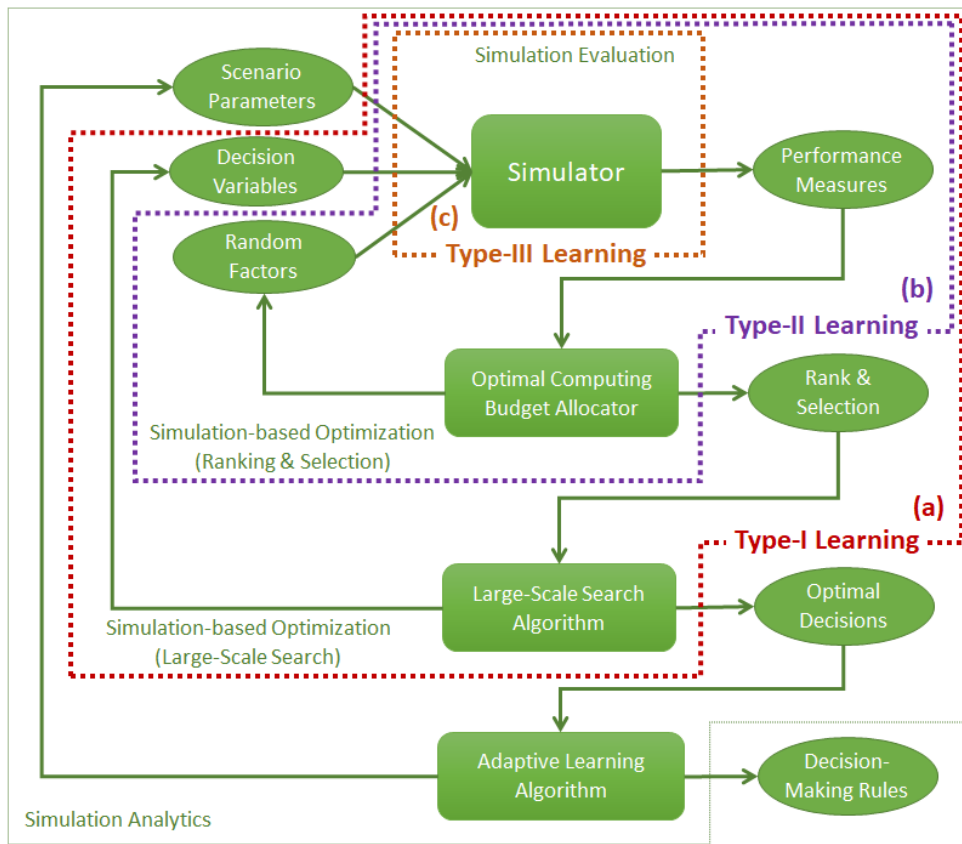


Figure 3: The four types of learning in simulation analytics.

6 COLLABORATIVE DEVELOPMENT

The new problems proposed could not be solved in one action or by a single group of researchers or research institutes. We need different researchers and organizations to collaborate in order to suggest and accomplish an entire ecosystem of smart digital twins that aggregates all functions of simulation, optimization, and learning. These include higher learning institutes, research institutes, equipment and platform developers, solution and system integrators, and end-users, etc. They will contribute to the final solutions at the different layers. We attempt to use the following pyramid to describe their relationships and roles of various collaborators, as shown in Figure 4.

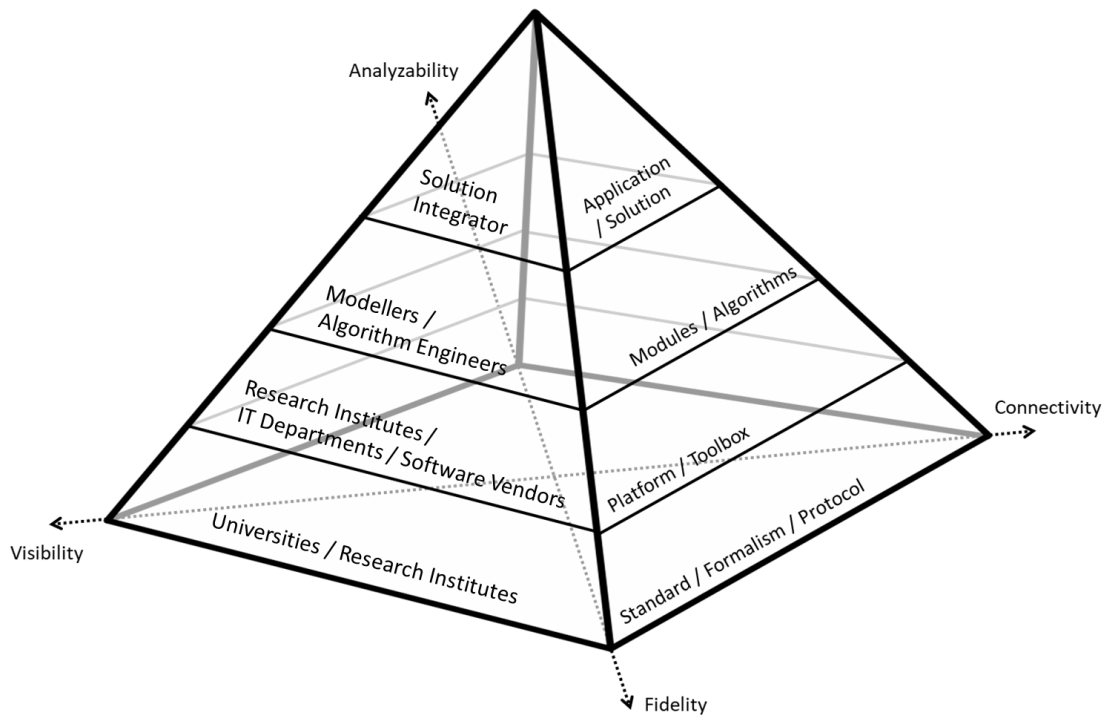


Figure 4: The collaboration pyramid for the three-carriages ecosystem.

At the bottom layer, we need to identify a system of standards, formalism, and protocols to normalize the simulation modeling, execution of simulation evaluation, and interaction between simulation modules and with optimization and learning algorithms, considering various computation infrastructure. In such a way, we could break out the boundaries between different programming languages and development environments. Such normalization could benefit the compatibility and communication between various components, enable the modelers to focus on the description of the detailed business logic of the industrial systems, and algorithm developers to focus on the improvement of algorithm efficiencies with the development tools they are familiar with. Some efforts at this layer include simulation modeling formalism, high-level architecture (HLA), and the framework of integrated simulation and optimization. As the development at this layer is across platforms and tools, they require a large number of efforts on the fundamental research in theories and thus suitable to be initiated by the universities and research institutes.

On top of it, there is a need for software tools and platforms to realize the norms established at the bottom layers, which makes it possible for developers to use them for modeling building and algorithms development that conform with the standards, and properly manage them. These platforms could base on one or several programming languages; alternatively, they could also adopt a graphical language or a system

of algebraic notations. No matter in which kinds, as long as the standards of the bottom layer are conformed, the simulation model built, and algorithms developed shall be compatible to each other. However, due to the difference in the tools, the developer-experience and development efficiency can deviate a lot. For example, the programming package we are developing now includes O2DESNet, o2despy, and O2DESNet.RCQueues can be categorized into the effort of this layer. The universities and research institutes can create such tools and platforms for academic research and educational purposes; alternatively, commercial companies could also undertake it to support other profitable projects.

Researchers and developers could build the simulation modules and analytical algorithms according to various domain problems with the software tools and platforms created. As all the components are developed on the platform that conforms to the standards, they shall all have compatible interfaces for common computational infrastructures. Therefore, they can be adapted to run collaboratively for simulation evaluation and decision analysis. The simulation modules on the platform will consolidate the domain knowledge in specific industrial sectors and sub-systems; meanwhile, the algorithms on the platform could also accumulate rich experiences from algorithm developers and engineers. All the components on the platforms can be reused and assembled in different analytical and intelligent decision-making problems which could be continuously validated and improved through wide applications. The platform could provide certain mechanisms to benchmark and feedback to the developed components, to provide version control functionalities, to manage the intellectual property (IP) dependencies, the trading system for the IPs as well as software licenses. Such mechanisms will potentially create positive feedback loop between academic research and industrial practices.

Ultimately, the suitable simulation modules and analytical algorithms can be selected and assembled by the solution integrator and applied for a specific domain problem. The final solution integrators can be researchers, consultants, or the IT departments of commercial companies. They are the ones who have a comprehensive understanding of the high-level structure of the system problem, but not necessary to be the developer or expert in each component of the simulation module or intelligent algorithms. As the roles are clearly defined, a team of known or unknown collaborators who are experts in their own domain will accomplish the smart digital twin solutions with high quality and efficiency.

7 CONCLUSION

This paper summarizes the functionalities and roles of simulation, optimization, and learning for intelligent decision-making on the background of Industry 4.0. The future research direction resulting from such trends are proposed. From our perspective, the decoupled real-time decision-making process benefits from the aggregation of optimization and learning. It provides the additional potential for applying simulation-based approaches in solving problems with complex industrial systems. The integration of the three essential technologies enables the general infrastructure of the smart digital twins. Meanwhile, it triggers a new requirement for the further development of the simulation methodologies.

Therefore, in this paper, we propose the technologies we are developing to tackle this issue. Simulation is enabled by the proposed technologies to play an important role in depicting the system models, generating data for optimization and learning, and validating optimized decisions and learned rules. And with technologies explored, we illustrate potential academic research problems and the directions for engineering development. A framework of collaborative development among various research institutes and companies is proposed at the end of the paper. We hope this work could serve as a valuable reference for the future development of simulation methodologies, as well as the deployment of smart digital twins and intelligent decision-making systems.

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