An Exploration of Frameworks for Modelling Cyber-physical Systems

Francesco Bondini[1] Felix Lagarden[1] Jakub Siemaszko[1], and Brian de Vrind[1]

[1] Delft University of Technology, Delft, The Netherlands
{f.bondini, f.r.lagarden, j.d.siemaszko, b.d.devrind}
@student.tudelft.nl

Abstract Cyber-physical systems (CPSs) combine physical processes with computational control systems and are used extensively in modern industry, transportation, and infrastructure management. Modelling and simulation of CPSs are crucial for the analysis, verification, and validation of such systems. CPS modelling faces challenges of system heterogeneity, time synchronization and concurrency, making the formal definition of such models difficult and often incomplete. In this paper, we analyse several existing frameworks for CPS modelling and highlight their limitations in the face of persistent challenges. In addition, we reason that existing generalized frameworks can be combined with domain-specific practices as an effective interim solution in the absence of a single internally complete, generalized modelling framework. The conclusion identifies a research gap and a recommendation for future work - the streamlining of coupling generalized frameworks with domain-specific practices.

Keywords: Cyber-Physical Systems · Modelling · Simulation · Framework · Concurrency · Heterogeneity · Synchronisation · Digital Twins.

1 Introduction

Cyber-physical systems (CPS) represent the intersection of computational and physical spaces and are commonly defined as the sum of physical processes, sensors, actuators and computational processes (Khoumsi, 2019). CPSs are an integral part of modern industry, with manufacturing (J. Lee et al., 2015; Weyer et al., 2016), transportation (Jia et al., 2016; Sampigethaya & Poovendran, 2012), healthcare (Zhang et al., 2017), infrastructure management (Hehenberger et al., 2016), and many other fields reliant on continuous and autonomous control of physical processes. With CPS often used in safety-critical environments, thorough modelling and simulation of such systems are crucial for verification and validation purposes. In addition, simulation of CPSs plays a vital role in their design, with real-time *digital twin* simulations often used as a reference for control systems (Gabor et al., 2016).

CPSs and their models face unique challenges, being immediate consequences of the interaction between the physical and computational spaces. CPSs face issues of synchronisation, system heterogeneity, and distributed system architecture. The modelling side additionally introduces the issue of implementation modelling (Derler et al., 2012), with features such as communication delays and data losses potentially impacting the model's accuracy. Facing these challenges, efforts have been made to define a coherent and abstract framework for CPS design. Nonetheless, the existing frameworks seldom address all issues faced by CPS and often do not account for the wide range of needs of various industries.

This paper aims to analyze existing frameworks for CPS modelling in search of common features, limitations, and strategies for handling common CPS challenges. Ultimately, we present this analysis to pave the way towards a unified, general framework for CPS models.

It is crucial to indicate the variety in possible CPS models, with a possibility for the entire system, or only its components to be modelled and simulated. A full CPS model would include a model for both the hardware and software domains, while hybrid models utilize one real-life component while modelling the other. In principle, both combinations result in valid CPS models. Throughout this paper, the focus is put on full CPS modelling, including both the computational and physical domains.

The remainder of the paper starts with an explanation of the literature study methods used in section 2. Then in section 3, a formal definition of cyber-physical systems is presented, along with a historical note. The section also establishes the most important challenges faced by CPS design, modelling, and simulation. The examined CPS modelling aspects are then presented in the following sections, including examples of digital twin implementations in section 4, attempts at generalized formal descriptions of CPS models in section 5, and an example of a domain-specific framework in section 6. Following, section 7 presents a comparison between the analysed frameworks, aiming to highlight their shortcomings and similarities and find approaches that have the potential to complement one another. Finally, relevant conclusions are drawn and presented in section 8.

2 Methods

The reference information for this review was gathered through desk research, focusing on the most impactful papers in the field of CPS modelling and simulation. The scope of the literature study included fundamental contributions to the modern understanding of CPSs, including their capabilities and challenges. A snowball method was utilized to identify the most impactful (most cited) papers in the field, focusing more strictly on modelling approaches.

The initial search revealed a vast range and depth of frameworks. As mentioned in section 1, we set out to compare the differences and similarities of these approaches. Hence keywords like "framework" and "formalism" were used to determine the first set of papers. The set was then filtered to find papers that described frameworks concerning different applications of CPSs, allowing us to compare how different applications may dictate a different structure of the model.

3 Cyber-Physical Systems

Historically, cyber-physical systems have existed since the early 1950s, with the introduction of the first digital computers (E. A. Lee, 2015). However, the term CPS has only been coined in the early 2000s, with Helen Gill often credited as the first proponent. She used the term in internal documents and research agendas, though not in formal papers. The first two heavily influential papers discussing CPSs are E. A. Lee (2008) and Rajkumar et al. (2010), both presenting the challenges faced by CPSs and several requirements for future systems and frameworks. These two papers are considered the fundamental papers that lay the groundwork for further reference works. Both authors are co-authors of several other papers that build on the fundamental ideas to define the modern understanding of CPSs.

CPSs have different proposed definitions in the literature, with a single formal definition not yet accepted within the field. Throughout this paper, we settle on the following definition, roughly encapsulating the existing interpretations: "Cyber-physical systems (CPSs) are physical and engineered systems whose operations are monitored, coordinated, controlled [...]." (Rajkumar et al., 2010, p. 731). In this definition, a CPS is any system interacting with the physical world through sensing and actuation, and using this interaction in control decisions.

The coupling of physical and computational domains is a subject of some ambiguity. In particular, the exact division point between the two is not well defined in the literature. The sensors and actuators are an important part of a CPS, however, they are not always defined as a specific component of the system. Oks et al. (2019) states that the sensor and actuator modules are part of the physical domain. Another option is to designate the sensors and actuators as the interface of the two domains, which is argued to streamline model verification (Hehenberger et al., 2016; Sampigethaya & Poovendran, 2012). No commonly accepted division between the physical and computational domains is currently accepted as standard, and the formal division of a CPS remains an open problem.

The study of CPS presents unique challenges as a consequence of the interlocking between the physical and computational space (Derler et al., 2012). Physical processes are inherently concurrent, which makes their management difficult within the typically sequential nature of software. This mismatch between CPS characteristics and their digital implementation can lead to potential conflicts and has to be rigorously addressed and managed during operation. From the simulation standpoint, the handling of concurrency carries yet another issue - the accurate modelling of concurrency in a (numerical) simulation of physical processes.

With the order of event handling often critical to the correct functioning of CPS, communication delays arise as a uniquely relevant aspect of such systems and their models (E. A. Lee, 2008). CPS models that ignore implementation features are often inadequate, with elements such as communication delays, networking protocols, data losses, and embedded hardware limitations significantly impacting the functioning of a CPS (Gabor et al., 2016). The modelling of implementation elements, as well as the joint dynamics between implementation and the intended functioning, are thus another crucial element of CPS modelling.

Finally, cyber-physical systems are inherently multidisciplinary, often combining vastly different high-fidelity systems under a single framework. This presents vast challenges in both design and modelling, as the domains can differ not only in jargon but also in the type of system formalism altogether. The combination of multiple, highly complex, and diverse subsystems makes the synthesis of CPS a difficult task and presents opportunities for unit, semantics, and transportation errors (Derler et al., 2012).

To address the issues presented above, several attempts at a generalized modelling framework have been proposed. Nonetheless, the wide range of domains covered by CPS often makes these attempts inadequate, as they struggle to combine the high level of abstraction needed to generalize the framework with the high level of detail required for industrial application (Derler et al., 2012). The remainder of the paper examines several existing frameworks, including both domain-specific and general approaches.

4 Digital Twins

Aside from verification and validation use, CPS models have the potential to be used at runtime of the system, acting as an additional source of information for control decisions. Using these *digital twins* (DT) can allow the system to make a vastly more informed decision, and, to some extent, utilise predictions of future events within the control loop.

In this section, we summarise two papers that, despite sharing a similar high-level structure, propose different implementations of a digital twin: Gabor et al. (2016) presents an implementation framework for a fully virtual model (modelling the entire system), while Semenkov et al. (2021) introduce the concept of the heterogeneous digital twin, combining modelled and real components.

4.1 Digital Twin as a CPS Component

Gabor et al. (2016) propose a high-level architecture for CPS utilising digital twins as part of the control loop. Of note, the authors use the term *cognitive system* for what in this paper is referred to as a computational system. The main difference between the two is that Gabor et al. (2016) place the physical hardware (the *controller*) as part of the physical domain instead of the computational system. The core of the framework introduced by Gabor et al. (2016) relies on treating the digital copy in the same way as the physical world. That is, the twin model should interact with the computational system through the same interface as physical inputs, effectively copying how the physical and cyber worlds interact.

In this framework, the computational system is explicitly divided into two parts - the *intuitive reactor* making snap decisions and handling safety-critical control events, and the *planner*, responsible for long-term optimisation. Gabor et al. (2016) argue for implementing digital twins in the planning component and present how these models can effectively interact with the same interface as the controller input/output using publish/subscribe messaging. In this implementation, a digital twin is capable of aiding control decisions by acting as a prediction model for future states.

Aside from a high-level CPS structure, Gabor et al. (2016) present a tiered division of the control system, including physical constraints (tier 0), hardwired control (tier 1), intuitive reaction (tier 2), and planned, long-term reaction (tier 3). The authors argue that tier 0 and 1 information flow is crucial for the correct functioning of a digital twin, as these control elements cannot be altered dynamically by the software and carry essential information, such as the precision of sensors and actuators, and the underlying laws of physics. In this implementation, the restrictions of the interface between the cognitive and physical systems is copied to the interface with the digital twin.

4.2 Heterogeneous Digital Twin

Another example of Digital Twin (DT) is presented by Semenkov et al. (2021). In this paper, they propose the use of digital twins for validation, monitoring, supervision, and control of industrial processes. Semenkov et al. (2021) introduce the concept of *heterogeneous* digital twins which, compared to a virtual digital twin, combines virtual (modelled) components with real ones. The paper does not give a specific definition of real components: they are in general hardware or software that are identical to the system being simulated. According to Semenkov et al. (2021), this solution is by design more accurate than a virtual digital twin and, compared to full-scale test prototypes, it applies to various life-cycle stages of the industry. The paper states that a heterogeneous digital twin is one of the best options for modelling Cyber-Physical Systems.

The heterogeneous approach overcomes the difficulties of modelling CPS by reducing the number of virtual components and, therefore, the number of components to be modelled.

Semenkov et al. (2021) proposes a high-level architecture for CPS, with the use of nested containers to define the structure of the real system and its digital twin. This simplifies the task of maintaining the equivalence between the two systems. Additionally, the container hierarchy allows for implementation at different stages of development.

Semenkov et al. (2021) also introduce a structure for configuration description. In the paper, the word configuration refers to "a set of backbone components (hardware and software) currently installed in the system" (Semenkov et al., 2021, p. 8). The configuration of the system is the set of configurations of each component, resulting in a configuration tree of the system. Thus the configuration is the key element whose equivalence with the real system must be preserved.

5 Formal Frameworks for CPS Modelling

The topic of abstract framework definition for CPS has been a subject of extensive academic work. A general framework that addresses all inherent challenges of CPS models is highly sought after, as modern CPS design often relies on domain-specific practices and differing jargon. Here, two such formal frameworks are presented and analyzed, highlighting the issues of heterogeneity, time synchronization, and domain interactions of CPS models.

5.1 Abstract Semantics for Heterogeneous Modelling

The inherent heterogeneity of cyber-physical systems makes it challenging to combine models into a unified high-fidelity system. The issue of subsystem interactions is often addressed by introducing and enforcing common jargon, syntax, and overall structure of the model. E. A. Lee (2010) argues that such an approach is inadequate (or, at least, insufficient) to create a unified framework for heterogeneity.

E. A. Lee (2010) proposes to embrace the diversity of different models and instead handle their coupling with the use of overarching architecture. The presented framework describes a system divided hierarchically into *actors* connected using *relations*. The strength of this structure lies in the abstract nature of actor interactions, allowing different methods-of-computation domains (MoC's) to coexist within a system. In the `Ptolemy II` implementation described by Lee, each actor can be part of one of many MoC domains, including discrete-event, continuous-time, or process-network domains. The interactions between domains are handled using director objects (both local domain directors and top-level model directors) (E. A. Lee, 2010).

The framework of E. A. Lee (2010) also addresses the issue of concurrency with a well-defined model of global simulation time. The author presents a time represented as a tuple: (t, n), where t represents physical time (in principle, any real value) and n is an indexing variable (integer) used to resolve concurrency. This simple model addresses many synchronisation issues resulting from concurrent events, in particular, the causality and ordering of events in a single time instant are both trivially handled in this representation. In addition, the inclusion of local directors allows for an implementation of local time, allowing for more freedom for submodels.

5.2 System of Systems Approach to Formal CPS Modelling

A possible problem when modelling a CPS is that while the computational segment is always a discrete system due to the inherent nature of software, the physical system can either be discrete or continuous in time. To be able to differentiate between the two cases K. H. Lee et al. (2015) introduces the notion of "Hybrid CPS" when the physical system is a continuous system in time and a "DES CPS" for which both the physical system and the computational segment are discrete in time. While a single, joint DES model can simulate the latter, the former is more complicated.

In a Hybrid CPS, the physical system can be modelled following a different formalism specific to the continuous time domain, while the computational segment can be modelled using a discrete formalism like DEVS (Concepcion & Zeigler, 1988). The advantage of using separate formalisms is that specific simulation engines exist for each formalism, which can be applied to simulate the created formal models. The disadvantage is that a communication layer needs to be added between them to synchronise time across the models and translate data from one model input format to another. For this K. H. Lee et al. (2015) introduces four Interface Functions.

Specifically, according to K. H. Lee et al. (2015), events in one discrete model can cause events to trigger simultaneously in other discrete models. Similarly, an event in a discrete model can start the emission of a continuous-time signal to a continuous model. When transmitting a continuous-time signal from one model to another model, it is transformed as a continuous function from the initial to the target signal instantaneously at each time t. Lastly, when transforming a signal to an event it is necessary to define a value for the signal to attain or pass. The specified event is then emitted at the exact time instant, that this value is reached.

6 Demonstrator Framework for Industrial CPSs

Oks et al. (2019) state that the increasing complexity of systems and indeterminate boundaries of such systems, increase the challenges of designing industrial CPSs (Oks et al., 2019). Oks et al. (2019) present a reference architecture that can be used to develop a model of industrial CPSs. This reference architecture seems to be aimed at engineers working in the industry instead of academics. This is a different target group that this paper is trying to reach, than the previous papers presented.

The reference architecture presented is designed for demonstrators of industrial CPSs. The demonstrators are intended to replicate and visualize the characteristics of the industrial CPS. The design elements of the demonstrators are derived from the actual CPS.

The reference architecture is split up into categories: objectives, components, attributes, demonstrator, scenario and the configuration (Oks et al., 2019). The objectives are the goals which are desired from the demonstrator. These can differ from demonstration and understanding to qualification, etc. The components are the different parts of the model of the CPS that need to be prepared to run the simulation. The attributes are the characteristics of the components. The model behaviour will change by altering the attributes, and the simulation will yield different results. The scenario has two main components: setting and users. The setting describes the demonstrator's use case and the method by which it is applied. The users represent the staff and stakeholders of the CPS.

This method of reference architecture gives a clear structure in all the different components and the decisions that also come with these. The components are all given a specific job and work together to make the model of the CPS. The attributes describe how the components are designed and how they work together (Oks et al., 2019). These attributes then also determine how the components together form the model.

7 Discussion

The reviewed literature presents an overview of the modern state of CPS modelling and simulation, covering common simulation type(s) (Gabor et al., 2016; Semenkov et al., 2021), attempts at formal framework definition (E. A. Lee, 2010; K. H. Lee et al., 2015), and domain-specific frameworks (Oks et al., 2019). In this discussion, we examine how these frameworks handle the challenges of CPS modelling introduced in section 3 and compare the commonalities, limitations, and scope of each approach. Subsection 7.1 focuses on individual assessment of each paper. Following, subsection 7.2 compares the findings and presents an overview of the similarities and limitations of examined frameworks.

7.1 Individual Models

The framework presented by Gabor et al. (2016) is a surface-level architecture that fails to address many challenges of designing and implementing digital twin models. The discussion is also limited in scope, ignoring issues such as real-time updates to the digital twin, or interactions between multiple parallel twin models. Given that these models require accurate modelling of an entire CPS with high fidelity, issues are also likely to arise with model complexity and associated computational cost (after all, digital twin simulation has to resolve in real-time). The architecture proposed by Gabor et al. (2016) does not attempt to solve these issues, instead only briefly listing components which should be modelled by the digital twin - the physical phenomena being sensed and actuated, the hardwired control elements and the interface between hardware and the computational system.

Similarly, the architecture presented by Semenkov et al. (2021) is vague and does not provide solutions to many challenges of CPS modelling. For example, the authors share, without suggesting possible fixes, the difficulties found in the synchronisation of the virtual environment because of the lack of papers discussing virtual environment timekeeping. The paper ultimately describes a specific application of a heterogeneous DT in detail without suggestions for extending the detailed structure to a more general case.

The framework presented by E. A. Lee (2010) is a high-level, yet detailed architecture for implementing diverse submodels in a single high-fidelity model. The formal description of data flow and interactions between models of arbitrary MoC is undoubtedly a powerful tool in CPS design and modelling and has since been proven effective in that application (Derler et al., 2012). Nonetheless, the abstract semantics described in the paper by E. A. Lee (2010) are, by design, incomplete, and do not describe the design of individual model components.

On the other hand, the formal model presented by K. H. Lee et al. (2015) is extensive and general. A small limitation of this formalism is that it does not allow for including a time delay in its Interface Functions. This time delay can, in the real CPS, be caused by either a communication delay between physically distant computational segments or due to conversion time from a discrete event to a continuous, analog signal and not modelling the time it takes to translate from the physical to the computational segment can lead significant reductions in simulation accuracy.

Differently from the other papers, Oks et al. (2019) presents a unique view on the industry application of Cyber-Physical Systems. This different perspective results in a different approach to modelling CPS, which is helpful since it gives insight into the application of the modelling of CPSs.

7.2 Model comparison

The examined papers all agree that the construction of a reliable CPS model relies on the careful integration of its fundamental components. These components, which serve as the building blocks, are critical for accurately representing and simulating the interactions between physical processes and computational systems. The formal CPS frameworks (E. A. Lee, 2010; K. H. Lee et al., 2015) both introduce a similar hierarchical structure , where atomic models are combined into larger composite models. While the terminology used in the literature may vary, this general structure remains consistent across different frameworks. The hierarchical approach is effective, as it allows for the breakdown of complex systems into manageable and, crucially, *reusable* submodels, streamlining model construction, analysis, verification and validation.

The examined literature highlights model heterogeneity as a crucial part of CPS modelling. CPSs often encompass submodels utilizing different methods of computation, such as discrete-event, continuous-time, and process network domains (E. A. Lee, 2010). The ability to support and integrate these heterogeneous submodels is critical for developing a comprehensive and accurate CPS model. The abstract frameworks handle heterogeneity through the use of hierarchy and subdivision, as well as careful formal definitions of atomic models and their relations, allowing for a general and coherent description of their interactions.

The hierarchical approach also addresses the issue of high accuracy requirements. With CPSs often encompassing complex, distributed systems, the need to accurately resolve individual components and their connections is crucial for model accuracy. With this requirement in mind, digital twin models shine as the most accurate CPS modelling approach, being a high-fidelity copy of the original system. Additionally, the introduction of real hardware components in digital twins (*heterogeneous digital twins*) can provide a way of forgoing implementation modelling altogether, often making heterogeneous digital twins more accurate than fully virtual models (Semenkov et al., 2021). Nonetheless, CPS models, and digital twins especially, often struggle with challenges plaguing CPSs, such as time synchronisation issues.

The presented frameworks potentially also introduce entirely new issues for CPS modelling. The abstract semantics presented by E. A. Lee (2010) are by design not complete and do not present a coherent modelling structure. Inherently, the abstract semantics are meant as a backbone for more domain-specific design guidelines. The formal approach of K. H. Lee et al. (2015) additionally acknowledges the added complexity of formally describing a CPS model, which may potentially dissuade the industrial use of formal modelling.

Presenting an alternative view, Oks et al. (2019) discusses a domain-specific framework for industrial applications. In this structure, the focus is put on practical application of CPS as opposed to creating a general overarching structure. The paper suggests an architecture that neglects points such as model hierarchy and subdivision, instead presenting a *checklist* for the required CPS components. Despite the obvious limitations of this approach, this example acts as a complement to the generalized frameworks and explicitly addresses their shortcomings.

The combination of these approaches, with a hierarchical high-level framework and domain-specific submodel definition shines as a potentially complete CPS model, addressing the issues of heterogeneity, time synchronisation, and specificity. We argue that, in the absence of an internally complete generalized framework, this approach could prove effective in CPS modelling. Nonetheless, the inherent reliance on domain-specific guidelines is acknowledged as a limitation of this hybrid scheme. The coupling of approaches is likely to result in conflicts, as differing jargon and the added workload of formal implementation may dissuade industrial implementation of formal modelling. This conclusion highlights a potential knowledge gap and a recommendation for further research, streamlining the integration process between industry-specific practices with abstract formal frameworks for CPS models.

8 Conclusions

The modelling and simulation of cyber-physical systems (CPSs) is a crucial part of the verification, validation and design of such systems. Modelling and simulating a CPS poses many challenges, most inherently related to the coupling between physical and computational domains. This paper sets out to examine and compare several existing frameworks for CPS modelling, in search of potential future improvements and research gaps.

The examined literature covers a variety of modelling aspects for CPSs, including examples of digital twins as a common high-fidelity CPS simulation type (Gabor et al., 2016; Semenkov et al., 2021), attempts at generalised high-level structure formalism for CPS modelling (E. A. Lee, 2010; K. H. Lee et al., 2015), and an example of an industry-specific framework with elements of submodel design (Oks et al., 2019).

The examined frameworks generally agree on the overarching hierarchical structure of a CPS model, allowing for streamlined reuse of individual submodels in analysis, verification and validation activities, as well as facilitating heterogeneous modelling. The complexity of such architecture is handled through a formal definition of atomic models and the relations between them. In principle, the formal approach allows several methods of computation to interact within one model. Nonetheless, the time-consuming and complex implementation of formal semantics is highlighted as a potential limitation of this approach.

Complementary to these frameworks, the various domain-specific guidelines act as detailed and practical approaches for low-level modelling. As such, we highlight the combination of abstract high-level architecture with low-level domain-specific design as a potential interim solution for CPS modelling in the absence of an internally complete high-level framework.

Nonetheless, this hybrid solution likely introduces new challenges, such as conflicts between industrial practices and the requirements of formal frameworks. We identify these challenges as a potential research gap and recommend further work to streamline the coupling between existing generalized modelling frameworks and industry-specific practices.

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