# HYBRID SIMULATION FOR CYBER PHYSICAL SYSTEMS –

# A PANEL ON WHERE ARE WE GOING REGARDING COMPLEXITY, INTELLIGENCE, AND ADAPTABILITY OF CPS USING SIMULATION

Andreas Tolk
The MITRE Corporation
903 Enterprise Parkway #200
Hampton, VA, USA
atolk@mitre.org

Fernando Barros
Department of Informatics Engineering
University of Coimbra, Pólo II
PORTUGAL
barros@dei.uc.pt

Andrea D'Ambrogio
Dept. of Enterprise Engineering
University of Rome Tor Vergata
Via del Politecnico 1, Rome, ITALY
dambro@uniroma2.it

Akshay Rajhans & Pieter J. Mosterman
Advanced Research & Technology Office
MathWorks
3 Apple Hill Drive, Natick, MA, USA
Akshay.Rajhans@mathworks.com

Sachin S. Shetty
Virginia Modeling Analysis & Simulation Center
Old Dominion University
1030 University Blvd, Suffolk, VA 23435, USA
sshetty@odu.edu

Mamadou K. Traoré
Université Clermont Auvergne
1, Rue de la Chebarde,
63178 Aubière Cedex, FRANCE
traore@isima.fr

Hans Vangheluwe
Department of Mathematics and Computer Science
University of Antwerp, Middelheimlaan 1
2020 Antwerpen, BELGIUM
Hans.Vangheluwe@uantwerp.be

Levent Yilmaz
Computer Science and Software Engineering
Auburn University
Auburn, AL, USA
yilmaz@auburn.edu

## ABSTRACT

During the Spring Simulation Multi-Conference 2017, a group of invited experts discussed challenges in M&S of cyber physical systems. This 2018 panel is a follow-on activity, asking how the combination of various simulation paradigms, methods – so-called hybrid simulation – can be utilized regarding complexity, intelligence, and adaptability of cyber physical systems. This paper is a collection of position papers of the participating experts, supporting their viewpoints represented in the discussion.

**Keywords:** hybrid simulation, cyber physical systems.

## 1 INTRODUCTION

Cyber physical systems (CPS) are generally defined *as systems with integrated physical and computational capabilities that can interact with humans through variety of modalities* (Baheti and Gill 2011). During the 2017 Spring Simulation Multi-Conference, Xiaolin Hu moderated a discussion of invited experts – Fernando Barros, Andrea D'Ambrogio, Pieter Mosterman, Hans Vangheluwe, and Bernie Zeigler – on "Challenges in M&S of Cyber-Physical Systems." While the 2017 panel focused on CPS as the object of

M&S activities, this panel has been asked to extend the discussion to the use of simulation as a computational capability of the CPS. As CPS are characterized by many new modalities and domains, they use many different modeling paradigms, methods, and solutions, which leads to challenges known to the M&S community from hybrid simulation approaches.

Even though the term hybrid simulation has been addressed in the simulation community since the 1960s, see, e.g., Burns and Kopp (1961), the use of the term changed over time. Early papers focused on the combination of digital and analog simulation, soon addressing the domains of discrete and continuous approaches (Cellier 1979). Other researchers were more interested in the mix of numerical and analytic models (Shanthikumar and Sargent 1983). Recent contributions often use hybrid simulation to address solutions using more than one modeling paradigm, combining agents, discrete event, and system dynamics. Mustafee et al. (2017) recommend addressing the whole spectrum as hybrid, allowing combinations on all levels of M&S categories: *"Hybrid M&S results from using two or more components of different M&S categories to generate something new, that combines the characteristics of these components into something more useful for the underlying M&S effort to be supported that are composable under the constraints of this effort."* These categories comprise qualitative and quantitative paradigms, methods developed within the paradigm, and techniques applying such methods over all abstraction levels, facets, and phases. This definition allows to address the new modalities and domains and resulting modeling paradigms, methods, and solutions observed in the CPS domain consistently.

CPS expose the characteristics of intelligent, adaptive, and autonomous systems, operating in complex environments, often in collaboration with other systems and humans. Simulation has a long-standing tradition within artificial intelligence methods often applied as a computational capability of CPS. How the use of simulation in general, and the use of hybrid simulation, will contribute to better managing the complexity and improve intelligence and adaptability of CPS is therefore one of the areas of interest to the hosting M&S and complexity in intelligent, adaptive, and autonomous system symposium.

This paper compiles the position papers provided by this year's experts addressing challenges and solutions, the state of the art of using M&S concepts in CPS, questions on complexity of such hybrid approaches, and lessons learned of general interest to the M&S of Complexity in Intelligent, Adaptive, and Autonomous Systems (MSCIAAS) community.

## 2 THE NEED FOR A UNIFYING FORMALISM FOR HYBRID SYSTEMS (BARROS)

### 2.1 State of the Art in M&S

Co-simulation has its roots in the work on hierarchical and modular models introduced in (Zeigler 1984) where the concept of abstract simulator was introduced to enable the independent simulation of discrete event models. Unfortunately, the representation of continuous systems did not accomplish the sound description that was achieved for discrete event models. Currently, modeling formalisms for continuous systems still rely on the nowadays extinct analogous machines (Burns and Kopp 1961) and they were not updated to reflect the ubiquity of digital computers (Henzinger 1996). The representation of continuous systems on a digital computer while enabling their co-simulation is currently a major research challenge.

### 2.2 The Need for an Explicit Representation of Numerical Methods

Ordinary Differential Equations (ODEs) play a key role in the representation of continuous systems. Conventional ODEs numerical integrators require the transformation of arbitrary order ODEs into a large system of $1^{st}$-order equations that is commonly solved by a single integration algorithm. Thus, the prevalent approach does not promote model independence and it does not provide the basis for co-simulation. Co-simulation requires the development of new methods. Quantization (Zeigler and Lee 1998) achieved a representation of $1^{st}$-order integrators in a modular form, enabling the co-simulation of hybrid systems. Unfortunately, conventional $1^{st}$-order integrators do not provide the best approach to solve all types of

ODEs. Other kinds of numerical methods have been developed to solve different families of ODEs. Geometric integrators are fundamental to represent 2nd-order energy preserving systems that need to be simulated for long periods. Examples include celestial mechanics systems, where simulation times of thousands or millions of years can be required. Other types of integrators can address stiffness using analytical approaches. This is the case of integrators that seek solutions in the form of exponential functions instead of using conventional polynomial interpolation.

Albeit important, ODEs do not have the exclusivity in system's representation. In particular, hybrid systems require the ability to combine ODEs with models that generate a discontinuous behavior. Examples include hybrid function generators, zero-detectors, digital controllers and digital filters. Additionally, hybrid systems are affected by pathological problems that include chattering and Zeno-behavior. To succeed, the co-simulation of cyber-physical systems need to tackle all these issues, while guaranteeing a sound semantics for achieving a deterministic simulation. Given the diversity of requirements, the problem of finding a unifying co-simulation representation for hybrid systems seems an overwhelming task. We consider, however, that an approach based on a reduced set of sound operators may provide the best solution to establish a general co-simulation framework.

### 2.3 A Unifying View of M&S

The Hybrid Flow System Specification (HYFLOW) formalism provides a description of modular hybrid models that combine sampling (Barros 2002) with discrete events (Zeigler 1984). HYFLOW models can be independently simulated being the interaction based on message passing that guarantees model encapsulation. HYFLOW co-simulation is supported by two basic operators: the ability to exactly represent dense outputs on a digital computer and the concept of generalized sampling (Barros 2002). These constructs have shown to provide the basis for describing a large variety of numerical methods, including 1st-order, 2nd-order (geometric), and exponential ODEs integrators (Barros 2017b). HYFLOW can represent PID digital controllers and sliding-mode controllers, a solution for achieving chattering-free representations (Barros 2017a). HYFLOW can also describe digital filters, zero-detectors, and Fluid Stochastic Petri Nets (Barros 2015, Barros 2016b).

HYFLOW provides a new approach to the representation of models described in multiple paradigms. Instead of treating models as heterogeneous, HYFLOW promotes a unifying view where all models are regarded as a realization of the basic HYFLOW model. The interoperability is guaranteed by construction, since models share the same underlaying description. The semantics of Sampled-based Systems was established through the definition of the equivalent I/O System in (Barros 2002). HYFLOW co-simulation algorithms for both atomic and composition levels can be found in (Barros 2016a).

### 2.4 Impact on Complexity, Intelligence, and Adaptability of CPS

The seamless integration of HYFLOW models can contribute to the representation of complex CPS based on different types of models that traditionally have been regarded as non-interoperable. This lack of interoperability would make it difficult, for example, to compose FSPNs with sliding-mode controllers, imposing, in many cases, a simplified representation of complex systems. Since the co-simulation of HYFLOW models is guaranteed, the interoperability of new families of models can be achieved by expressing these new models in the formalism. HYFLOW also provides the ability to dynamically change model composition. Dynamic topologies make it easier to express adaptable CPSs that modify the interaction between components, or even that change dynamically their set of components. The HYFLOW reflective nature makes it possible to improve model intelligence by enabling model topology to be used as a decision factor.

## 3 MODELING METHODS FOR HYBRID M&S OF CPS (D'AMBROGIO)

CPS are characterized by an unprecedented ensemble of heterogeneous and distributed elements, such as sensors and actuators, as well as more complex devices such as computers, self-driving vehicles, and autonomous robots. The heterogeneity and complexity of modern CPS embrace both software and hardware, not mentioning the humans-in-the-loop, thus making CPS difficult to describe, understand, predict, manage, design, and/or change. Such difficulty mostly stems from the fact that the CPS engineering involves building, implementing and executing heterogeneous models of heterogeneous components, from the early phases of the CPS lifecycle down to the operation and maintenance phase, with models being heterogeneous in terms of both formalisms and levels of abstraction (Mustafiz et al. 2016). The intelligent, adaptive, and autonomous properties of modern CPS contribute to look at them as truly *complex* systems (i.e., with emergent behavior and in presence of uncertainty) rather than as systems that are simply *complicated* because of their size and heterogeneity (Tolk et al. 2018).

The M&S community has provided effective solutions to deal with the single-formalism multiple-components case, and is being actively working to provide "holistic" solutions for dealing with the multiple-formalisms multiple-components case, as perceived by research and development efforts carried out in the *Hybrid M&S* field, with significant contributions in terms of parallel and distributed simulation and co-simulation, as well as in terms of multiscale, multi-paradigm, multi-resolution, and multi-physics modeling (Mustafee et al. 2017).

### 3.1 The composability challenges

It is my opinion that most of the challenges that we have to cope with in the Hybrid M&S field do not come from the "simulation" leg but rather from the "modeling" leg of a Hybrid M&S effort, with model composability being one significant example of such challenges.

*Model composability* can be thought as the capability to select and assemble modeling artifacts across different formalisms, levels of abstraction, and lifecycle phases into new artifacts, which are eventually translated into simulation systems that satisfy the M&S user needs. The topic of composability has been addressed in the M&S field both to define a formal theory of validity (Petty and Weisel 2003) and to provide pragmatic approaches that enable semantic and syntactic interoperability at simulation model building and execution time (Tolk and Muguira 2003).

I'm here focusing on such pragmatic perspective, as applied to exploit Hybrid M&S solutions in the CPS domain. The typical M&S users are thus CPS engineers in charge of carrying out V&V activities throughout the system lifecycle, in order to properly build and operate CPS that may require not only high efficiency, reliability, safety, and security but also regulatory compliance, scalability, adaptiveness, autonomy and serviceability. In this respect, the challenge is not only how to assemble heterogeneous simulation models and translate their representational format into executable simulations, but also how to guarantee a proper usability of the "composed" solutions, so as to support a wider set of application opportunities and M&S users, which should not be required to be aware of the complexity underlying such solutions.

### 3.2 Model-driven engineering as a candidate for meeting (part of) the composability challenges

Model-driven engineering (MDE) (Schmidt 2006) can help meet the challenges. The potential of MDE does not stand in the various incarnations that have been realized and applied, with diverse results, in the software engineering field mainly (being OMG's MDA a notable example), but rather in its inspiring principle, which focuses on the use of models to define and verify other models. According to the MDE perspective, each modeling language is centered around the use of a *single model*, which is often referred to as the meta-meta-model in the conventional metamodeling layered architecture (e.g., MOF in the MDA case).

What is conceptually needed to get the MDE benefits in terms of (1) automated approaches that enable the required interoperability and/or composability of Hybrid M&S solutions, and (2) reusability that enables sustainable solutions in terms of time, cost, and effort is achieving consensus on the adoption of a given meta-meta-model to define the modeling language (meta-model) of any types of model (e.g., hybrid models). This is the major strength but also the main practical limitation of current MDE approaches, since different incarnations of MDE principles refer to different meta-meta-models and thus call for alignment approaches. In the M&S field, MDE has been mainly used as an enabler for federated simulation (Gianni et al. 2008, Topcu et al. 2016).

In order to fully exploit the MDE potential in the field of Hybrid M&S for CPS, it is essential to augment the MDE theory with dynamically shared semantics and increased degrees of automation for model composability, by addressing significant challenges in terms of model definition across abstractions (design-time conceptualization vs. run-time unsupervised learning) and definition of multi-directional adaptive mappings with behavior semantics.

On the practical side, a parallel effort has to address the delivery of Hybrid M&S solutions that provide the expected usability, so as to bring already existing Hybrid M&S solutions for CPS, as well as new research findings, to the wide set of end users who do not have the resources, the expertise, and/or the skills to uncover them. MSaaS (M&S as a Service) is gaining momentum as an effective approach to bringing the benefits of service-oriented architectures and cloud computing into the M&S field, so as to enhance interoperability, composability, and reusability and reduce the costs of M&S efforts (Bocciarelli et al. 2013). MSaaS thus promises to be a good candidate for meeting the usability challenge, provided that additional research is carried out to address technical issues related to service packaging, service discovery, service composition and orchestration strategies, as well as non-functional properties such as security, privacy and sustainability.

# 4 CPS AS COLLABORATING SYSTEMS (RAJHANS AND MOSTERMAN)

Computation and communications have become the main drivers in increasing system functionality as well as complexity. To guide the discussion, we focus on adaptive and autonomous systems in the domain of computation, while for communication we concentrate on connected and collaborative systems. The corresponding behaviors and implications are discussed and the resulting M&S challenges derived.

## 4.1 A classification of engineered systems along Computation and Communication axes

Following the exponential growth curve of Moore's Law, computation has rapidly proliferated in engineered systems to incorporate ever-increasing functionality that reflects human cognitive functions. In a traditional control systems sense, such *adaptive systems* are able to interpret their environment and act directly based on the information gleaned. These systems are characterized on the one hand by the presence of a rich observation fabric in modalities such as sound, vision, etc., and corresponding sensor fusion for signal to symbol transformation while on the other hand presenting unique challenges that result from the adaptivity when ensuring safe operations among humans. Adaptivity supplemented by the ability to perform reasoning and planning tasks has been essential in the field of *autonomous systems*. Such systems are characterized by a large operational envelope because of typical mobility in support of autonomy and emerging behavior when operating in circumstances not specifically conceived in design but nominally included as intended behavior. A consequence of the range of technologies and disciplines that converge in these adaptive and autonomous systems is the introduction of a challenging level of heterogeneity in the different levels of integration across components and subsystems.

As information technology started to permeate business and society, computer networks became an increasingly important element with Metcalfe's Law now starting to supplant Moore's Law. The added layer of communication has ensembles of systems come online that share their observation knowledge as connected systems. Such *connected systems* often rely on the availability of wireless communication which is subject to resource constraints (e.g., battery charge, base station access) and different use (e.g., high throughput requirements on video vs. low latency requirements on information for control purposes).

Likewise, individual autonomous systems are extended into ensembles of *collaborative systems* (Mosterman and Zander 2016). This results in characteristics such as functionality being assembled at run time via online (re)configuration while attempting to meet rigid constraints on safety and security, and sharing of resources available in the collaborating systems in a manner that may require dispatch of functionality across compute platforms (e.g., a system with fully-charged battery may perform functionality in support of a collaborating system with less charge).

### 4.2 M&S Challenges

Given the inherent adaptivity of all of these systems, during their conceptualization the utility of physical test and experimentation is severely diminished so that virtual system engineering becomes a key technology in design. Moreover, to substitute for the value of physical test and experiment, the virtual worlds must attain a level of fidelity close to that of the physical counterpart for aspects under study.

Specific challenges in the operation of *adaptive individual* systems include the need to interpret their surroundings, which requires the ability to generate models online (e.g., Simultaneous Localization and Mapping, SLAM) as well as carefully calibrate generated or precompiled models.

For *autonomous individual* systems, the ability to operate in a broad range of environmental conditions requires robust sensing abilities. Here, models of sensors and sensor configurations are key to respond to changing conditions. Generally, challenges involve the necessity for online adaptation of system architecture as well as switching variants of functionality and for handling different quality of service (QoS) constraints possibly in the face of degraded service circumstances all while relying on performance models to operate in an optimal sense.

When systems operate as *connected ensembles*, communication models address the challenging need for varying levels of QoS between different network nodes and for different purposes so as to effectively configure the protocol stack. Moreover, embedded applications often are of a demanding real-time nature and require highly precise timing between network nodes. Finally, sharing data as information builds on models of data and ontologies to allow meaningful exchange.

For operating *collaborative ensembles* of systems, sharing of behavior models is the foundation of effective coordinated activity to make explicit what an action will entail but also how another system may repurpose behavior to achieve a different goal (i.e., make the behavior functional). Success mandates formalized assumptions on when the model applies. Methodologies to determine function in the face of concurrent resources put requirements on necessary advances in distributed planning and control synthesis.

In addition to challenges in the *operation* of systems, *design* embodies a set of challenges in its own right. Because of the difficulty in experimenting in a physical sense, the use of models is critical. The various levels of details and representations necessary for the range of tasks involved in design as well as the different representations across heterogeneous technologies requires model transformation to automatically arrive at a model that is proper for a given objective (Mosterman and Biswas 1999). Additionally, where model transformation does not apply (either for lack of power or because of lack of model availability) it is essential to either connect, combine, or integrate models in different formalisms. Throughout all of this, various dynamic and execution semantics are present for which efficient simulation models must be used (Mosterman 2007). Finally, tools and procedures across design stages and even more so across organizations present a heterogeneous ecosystem (Rajhans et al. 2014). To enable consistent design, models must be projected to retain the aspects that are needed while maintaining consistent semantics implemented by different execution engines.

## 5 CYBER PHYSICAL SYSTEMS RESILIENCE (SHETTY)

Critical infrastructures such as, power grid, oil and gas refineries, water distribution are characterized by complex technological networks, and its cyber-physical interconnectivity presents a "surface" for cyber-attacks. The potential for disruptions in these critical infrastructures can be attributed to the dependence and the vulnerability of the networks interconnecting the physical plants and control centers. There is a need to develop cyber resilience metrics for these critical infrastructures to provide quantitative insights into ability of security controls to ensure operational resilience and development of cost-effective mitigation plan. It is highly unlikely for researchers to gain access to data from operational environments to generate resilience metrics. Instead, a hybrid simulation environment that characterizes both the cyber and physical environments would be applicable and provide useful cyber resilience metrics which can be useful for decision support systems and eventually help formulate an informed mitigation plan. Following are the challenges with developing hybrid simulations for Cyber Physical Systems Resilience

### 5.1 Fidelity

There is a need to strike a balance between the amount of details needed to characterize the components underpinning the cyber and physical infrastructure. The NIST Industrial Control Systems Reference Defense in Depth architecture provides a reference framework for critical infrastructure stake holders to protect CPS. However, this architecture has multiple layers and an attack on most of the higher layers may not lead to an attack on the cyber-attack. Hence, it is critical to include components in the simulator which would play a critical role in the cyber-physical attack. For instance, if the attack only results in the corporate network going offline, then this type of attack and the associated scenarios need not be included in the simulator. The components that can be exploited to launch multi-stage attacks which eventually lead to an attack on the physical plant should be given higher credence. The current state-of-the art efforts in modeling and simulating attacks on critical infrastructure mostly focus on local and cascading failures which are caused due to physical faults (Kinney et al. 2005). Specifically, researchers have simulated the critical infrastructure's structural resilience to deliberate physical attacks to plants, control centers, transmission lines, and communication systems. Physical attacks in contrast to cyber-attacks are deterministic in nature because attackers are aware of the system units to target. Due to the selective nature of the physical attacks, the impact felt on the immediate victims or potential of cascading events are not similar to cyber-attacks. The physical attacks are also characterized by temporal selectivity. The timing of physical attack is chosen to maximize the impacts. In contrast, the timing of cyber-attacks cannot be always guaranteed to be precise. The restoration process after a successful physical attack versus cyber-attack may have different timelines. These factors need to be incorporated in the hybrid simulations to the attacks will closely mimic the exploitability and impact of cyber-attack.

### 5.2 Effectiveness

Prior to developing the hybrid simulation environment for cyber resilience metrics, there is a need to develop a CPS resilience simulation framework. Tierney and Bruneau (2007), proposed a R4 framework for disaster resilience across the Technological, Organizations, Societal and Environmental (TOSE) dimensions. The R4 framework comprises of Robustness (ability of systems to function under degraded performance), Redundancy (identification of substitute elements that satisfy functional requirements in event of significant performance degradation), Resourcefulness (initiate solutions by identifying resources based on prioritization of problems), and Rapidity (ability to restore functionality in timely fashion). This framework does provide a starting point for development of cyber-physical resilience simulation framework. A hybrid simulation framework that will allow measurement of the R4 across the TOSE dimensions for cyber physical systems will address all the aspects that are required for CPS resilience. The ability to characterize the interplay between the TOSE dimensions will be crucial. For instance, merely computing the R4 metrics from the Technological dimension and organizational dimension independently will not provide effective insights into the lack of resilience. The R4 metrics in the Technological dimension would not be aware of the mission goals and organization constraints which will limit the effectiveness of the simulation and lead to silo effects. There are factors at the intersection of these four dimensions that need to be accounted for in a hybrid simulation framework. The hybrid simulation framework is only effective if it provides useful insights to not only the technology stakeholders, but also, decision makers, who would like to utilize the outputs from the simulations to develop informed decision support systems.

### 5.3 Actionable Intelligence

The purpose of developing the hybrid simulation framework for cyber physical system resilience is not only to generate quantifiable resilience metrics, but also, provide an action plan for mitigation to improve resilience. In order to improve resilience in CPS, the mitigation strategy could focus on the cyber or physical components. The hybrid simulation framework should be able implement both type of mitigation strategies and provide actionable intelligence on the effectiveness. In addition, the mitigation strategies should also be aligned with the TOSE dimensions to ensure that the proposed changes are not adversely impacting the interplay between the TOSE dimensions. Though there are several cyber focused mitigation strategies, they are typically dependent on the type of cyber component and are not amenable to generalized mitigation plans which are applicable to broader class of CPS. However, the physical systems do not undergo changes at the rapid pace at which cyber technologies evolve. Physical systems follow laws of physics and have inertia. We can leverage this property to find out if the physical systems can operate at an acceptable capacity even a signal is tampered or lost. There is considerable order of magnitude difference between physical and cyber speeds. The inertia property in CPS provides the latitude to operate even if some of the states are lost. Within the hybrid simulation framework, it will be beneficial to observe to what extent cyber-attack can be withstood, if the physical system can tolerate loss of signals. The simulation framework should be able to answer questions on detection (when should we drop), fault isolation (what should we drop), recovery (how soon can we recover to known good state).

## 6 MULTIPERSPECTIVE MODELING AND HOLISTIC SIMULATION (TRAORE)

### 6.1 From complexity to hybridization

Managing complex systems can be tedious (Simon 1972) not only because of a huge number of subcomponents that may compose them but also because of the complex processes that govern the relations that exist between them rendering their analysis and design more difficult. Modern complex systems like CPS require multiple levels of explanation be provided to achieve their various objectives, while keeping a holistic understanding of the behavioral pattern of the overall system and its interaction with the surrounding environment. As such, a hybridization of approaches that would evidently provide useful knowledge from various angles on how such systems perform at the holistic level rather than focusing on specific problems in isolation for specific solutions is an appropriate means to address their complexity. In Modeling & Simulation (M&S), such a hybridization can be envisioned endogenously or exogenously, and at different levels of concern. As described in Table 1, the concepts level, where the universe of discourse is set (such as the notions of state, event, concurrency…), calls for formalisms and (more generally) methods to capture the required concepts in a symbolically manipulatable way. While the M&S community traditionally distinguishes between discrete and continuous phenomena as regard to central time-related concepts, qualitative and quantitative computational approaches, such as Operation Research or Artificial Intelligence methods, rather focus on problem-solving steps and mechanisms. Hybridization comes at this level with the objective-driven need to deal with temporal considerations for the system under study while trying to find a solution to the problem under study. Such a situation happens for example when optimization techniques make use of simulation as a black box-type of evaluation function (exogenous hybridization), or when the requirement for a fine-grained understanding of the system entails both continuous and discrete phenomena be considered (endogenous hybridization). At the specification level, the real-world system and problem under study is expressed as a model, using the universe of concepts adopted, i.e., discrete or continuous simulation model (within M&S world) or problem-solving algorithm (within the wider computational world). The literature has coined various terms to qualify the various possible hybridizations, such as DisM + ContM, or DisM/ContM + Alg (where "+" denotes a composition/mixing operation that can vary from loose to tight integration). At the operations level, engines are built to execute the model defined at the immediate upper level. Such engines are often referred to in the M&S world as simulators and integrators (for respectively discrete and continuous operations), while solvers implement the algorithms defined in non M&S-centered computational approaches. Operational hybridization occurs here to support the requirement for multiple execution engines, each devoted to aspects that other engines do not support. The essence of CPS is the hybridization done at the operations level between computational engines and physical components. The hierarchy of levels in Table 1 implies stronger hybridization at the upper level and weaker hybridization at the lower level. Consequently, taking CPS challenges from the operations level to the models or even the formalisms level has the potential to provide the same benefits as Model-Driven Engineering aims at in systems engineering (Da Silva 2015).

**Table 1:** *Hybridization strategies in computational frameworks.*

| | | | | |
|---|---|---|---|---|
| ***Concepts*** ***(formalisms)*** | DEVS, Petri Net, Multi-Agents… | ODE, PDE, System Dynamics… | OR methods, AI methods… | |
| ***Specifications*** ***(models)*** | Discrete simulation models (DisM) | Continuous simulation models (ContM) | Algorithms (Alg) | |
| ***Operations*** ***(engines)*** | Simulators (Sim) | Integrators (Int) | Solvers (Sol) | Physical devices (Phy) |
| | M&S world (SimW) | | | |
| | Computational world (CompW) | | | |

DEVS: Discrete Event System Specification

ODE: Ordinary Differential Equations

PDE: Partial Differential Equations

OR: Operation Research

AI: Artificial Intelligence

----: often referred to as hybrid simulation

----: often referred to as combined simulation

----: CPS

## 6.2 The need for multiple levels of explanation in a holistic view

In a systematic view, a system of systems approach (Zeigler and Sarjoughian 2012) supports the modelling of large loosely coupled distributed complex systems that target the optimization at the macro level which is the entire system itself, instead of the micro component system level. However, it is a challenging task to model such complex systems and one has to carefully choose the levels of abstractions that fit into the holistic view of the entire system in order to gain multiple explanations and more efficient computational results. The "holy grail", as coined by Brailsford et al. (2010) is referred to as an approach that combines different other approaches to provide a truly holistic systems view. The multi-perspective modeling and holistic simulation (MPMHS) approach can provide a helpful framework for that search (Djitog et al., 2017a; Djitog et al., 2017b).

In practice, M&S processes are often identified from a given perspective and are executed in isolation, i.e., without recourse to the processes built from other perspectives. In reality, however, processes usually have mutual influences, which has a greater impact when it comes to complex systems like CPS, where "everything affects everything else" (Brailsford et al., 2010). However, building a monolithic highly detailed mega-model (that involve all inter-influencing factors) is not considered as viable (Brailsford et al., 2011).

To address this issue, MPMHS suggests a stratification of the levels of abstraction into multiple perspectives and their integration in a common simulation framework. In each of the perspectives, models of different components of the system can be developed and coupled together. Concerns from other perspectives are abstracted as parameters. That way, each perspective can be seen as encompassing a family of questions that can be formulated through dedicated experimental frames (Zeigler, 1984). Consequently, the resulting top model within each perspective can be coupled with its experimental frame to run simulations and derive results.

While this feature provides multiple levels of explanation for the same system, there is also the need to encompass the influences of perspectives on one another. To allow a holistic simulation, which encompasses isolated perspective-specific simulations and their mutual influences, without a drastic increase of complexity, we suggest an integration mechanism to enable live exchanges of information between models from different perspectives. While models within the same perspective are coupled the classic way (i.e., outputs to inputs) to form larger models within the same perspective, models from distinct perspectives relate in a different way. Indeed, the parameters of a focused model in a given perspective are fed by the outputs of models from other perspectives. In other words, these outputs provide a disaggregated understanding of the phenomena approximated by the parameters of the focused model. The resulting global model can be coupled with a holistic experimental frame to derive results that cannot be accurately addressed in any of the perspective taken alone.

The MPMHS approach has been formalized and applied to healthcare systems (Djitog et al., 2017a; Djitog et al., 2017b; Traoré et al., 2018). It is applicable to other forms of CPS as well.

## 7 MULTI-PARADIGM MODELLING (VANGHELUWE)

### 7.1 Complexity

The complexity of the Cyber-Physical Systems we (aim to) design and build is increasing in leaps and bounds. The main causes of this complexity are: the vast number of components, the multiple views on a system-to-be-built, by different stakeholders, the diversity of both components and views, often spanning very different domains (informational, physical, network, but also safety, sustainability and other ilities), leading to inconsistencies between views, the diversity of component interactions, uncertainty and partiality of knowledge, the perceived changing structure of the system (at some level of abstraction), emergent behaviour, often due to non-compositional interactions, and the complexity of the concurrent development processes, which often need to satisfy contradicting goals such as agility on the one hand and certification on the other hand.

For some of these causes of complexity, solutions have been devised and are commonly applied. The large number of components for example is tackled by constructing models hierarchically. This is only possible if the interactions between the components are highly structured, something which is often imposed "by construction" in engineering. Note that this implies that modelling languages, with well-defined syntax and semantics, support hierarchy.

### 7.2 Multi-Formalism Modelling and the Formalism Transformation Graph

For complexity caused by systems (hierarchically) composed of sub-models in different formalisms, some solutions exist. The meaning of such a multi-formalism model can for example be given if all component models can be transformed to a common formalism, preserving properties of interest (such as simulation traces). Once all components are in the same formalism, it becomes easier to reason about the meaning of their composition. This approach was formalised in (Vangheluwe and Vansteenkiste 1996). A Formalism Transformation Graph (FTG) as shown in figure 1 charting all possible formalism transformations can guide the modeler.

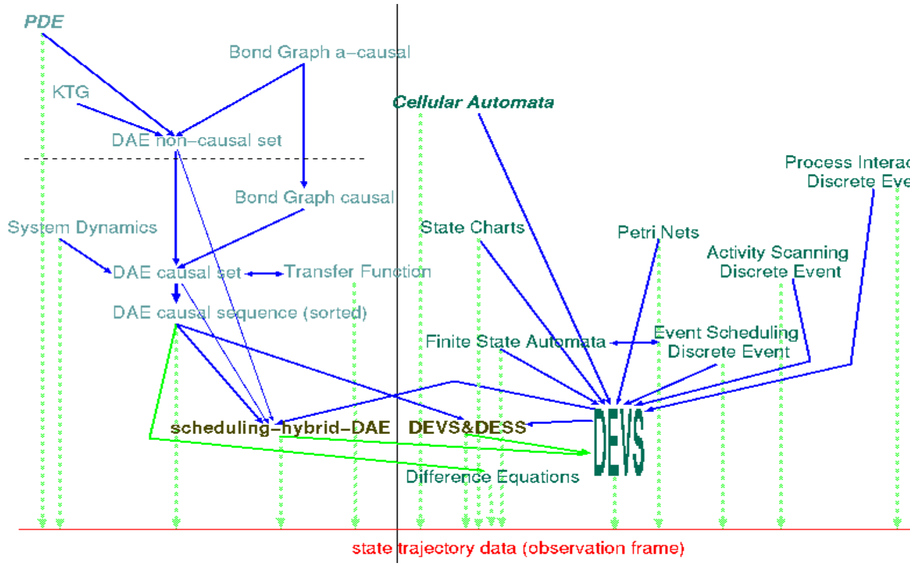


**Figure 1:** Formalism Transformation Graph (FTG).

The nodes in the FTG represent formalisms and the edges represent formalism transformations that preserve simulation results. The dashed lines denote the special "simulation" transformation, which generates simulation traces. Composition at the level of behavior traces or state trajectory formalism level, here represented as a horizontal line, is called co-simulation (Gomes et.al. 2017). In Figure 1, the solid vertical bar in the middle denotes the distinction between continuous-time formalisms on the left and discrete-event and discrete-time formalisms on the right. Transformations on either side are lossless w.r.t. simulation traces. Crossing the vertical bar from the left to the right entails an approximation however. Note that the DEVS formalism (Zeigler 1984) plays the role of the ultimate target of many transformation paths, as does the behavior trace formalism. As such, it acts as a universal simulation formalism. Note that Domain-Specific Modelling Languages (DSMLs) can be added to the FTG, with the semantics of domain-specific models given by mapping them onto a known general-purpose formalism.

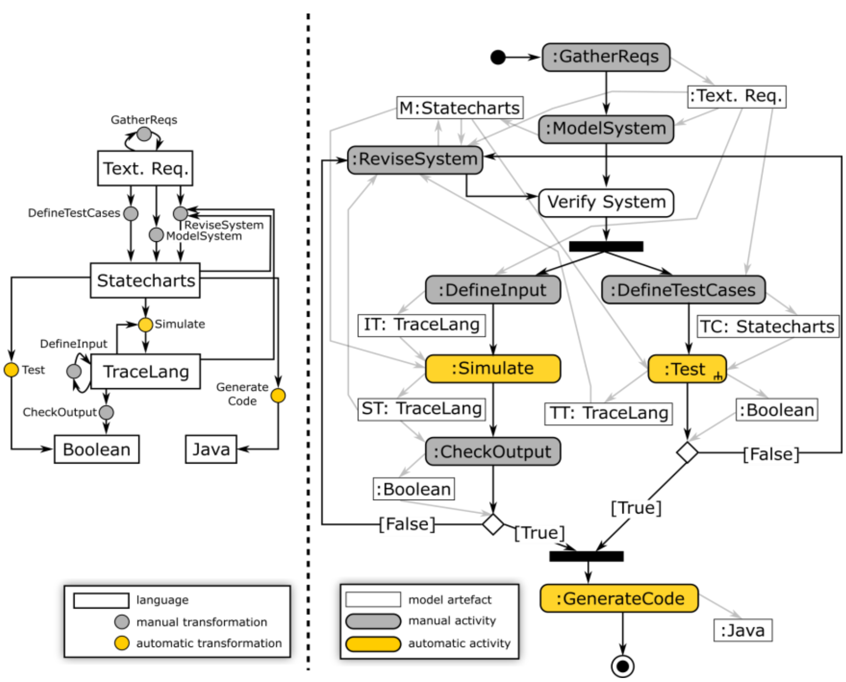


**Figure 2:** Formalism Transformation Graph + Process Model (FTG+PM).

As the model development processes become more complex, the need arises to explicitly model them. This leads to a Formalism Transformation Graph + Process Model (FTG+PM) (Lucio et.al. 2013). Figure 2 shows an example FTG+PM for the development of statechart models for timed, reactive systems.

On the left-hand side, the FTG shows the formalisms used: Textual Requirements, Statecharts, simulation Traces produced by running a Statechart simulation, Boolean, as a result of running a test (an encoding of the Textual Requirements in the form of Statecharts), and Java code synthesized from the Statechart model. The edges of the FTG depict the possible transformations between formalisms, either manual or automatic. On the right-hand side, a PM depicts the workflow, in the form of an Activity Diagram. The round-tangles are activities, and are the realizations of the corresponding transformations in the FTG. The rectangles denote artefacts that are input/output to the activities. They are typed by the corresponding formalisms in the FTG. There needs to be a morphism between FTG and PM. The PM in the figure depicts some iterative process whereby textual requirements are the basis for either manual simulation or automated simulation-based testing, in a feedback loop, ultimately leading to generated Java code. A PM can be used in a descriptive fashion, documenting existing processes or in a prescriptive fashion, as a basis for enactment.

### 7.3 Multi-abstraction and Linguistic/Ontological Modelling

Certain questions, such as whether a system is safe, are best answered at a high level of abstraction, either because only limited information is needed/available, or because analysis techniques such as model checking do not scale to models with the full amount of detail typically used for simulation. This means that some of the transformations in the FTG may not preserve all properties. Indeed, the essence of abstraction is that only some properties are preserved. When development processes become concurrent, with multiple activities taking place at the same time, possibly by different stakeholders in different domains, managing model consistency becomes crucial. Here too, abstraction can be used.

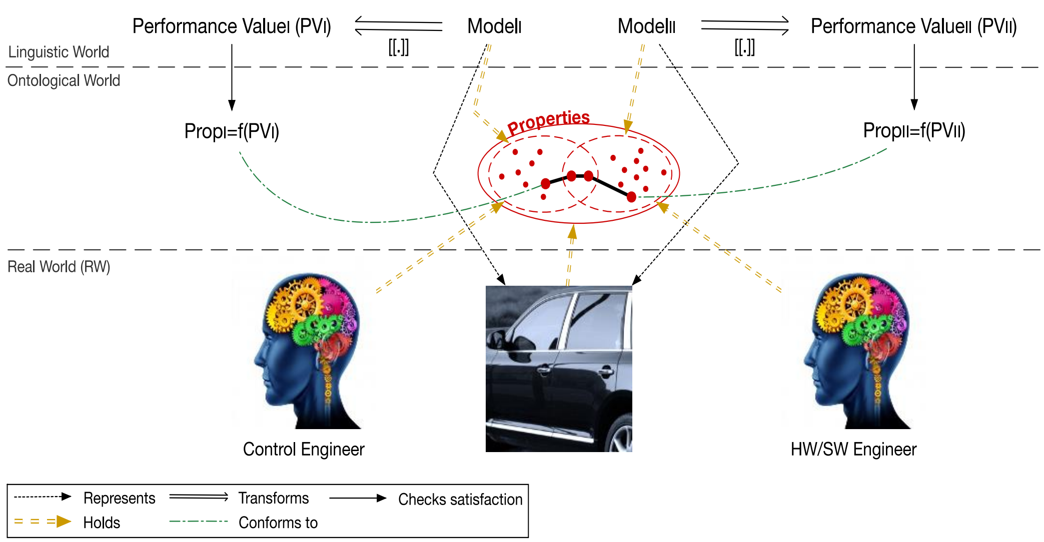


**Figure 3:** Linguistic and Ontological Modeling.

As shown in Figure 3, different engineers such as a control engineer and a Hardware/Software engineer may work on designing (different aspects of) the same car power window system (Vanherpen et.al. 2016). The individual engineers use their own modelling languages (aka "linguistic models") for which a semantic mapping function [[.]] exist which gives (for example, trace) semantics. The semantics of these models can be used to obtain performance values (such as total energy used), which in turn can be used to check the satisfaction of "linguistic" properties such as "is energy efficient", obtained by comparing the performance value with a threshold. As the two engineers do not know each other's domain, they may change their models in inconsistent ways. Linking the properties through an "upper ontology" locally relating properties, may reveal inter-disciplinary dependencies.

### 7.4 Multi-Paradigm Modelling

The above form a basis for Multi-Paradigm Modelling (MPM). In MPM, complexity is tackled by *explicitly modelling all* pertinent information, at the most appropriate *level(s) of abstraction*, using the most appropriate *formalism(s)*, with *processes* explicitly modelled too (Vangheluwe et.al. 2002). To define MPM, the notion of "paradigm" must first be given. A paradigm *P* is a collection of formalisms/languages, abstractions, and processes that satisfy properties that are considered characteristic for *P*. The Object-Oriented Paradigm (OOP) for example includes formalism(s) that have notions of object identity, of encapsulation, of specialization, etc. Abstractions/formalisms such as UML class diagrams, but also programming languages such as Java satisfy the OOP properties. Processes such as the Rational Unified Process also satisfy OOP properties such as being iterative. Defining paradigm as above intentionally (as opposed to extensionally), in terms of properties, has the advantage of being executable, in the form of a decision procedure. With this definition, "multi-paradigm" follows naturally, as a collection of formalisms/languages, abstractions and processes, composing these of the individual paradigms, while satisfying some combination of the individual paradigms' properties. This breaks down to composing formalisms/languages, abstractions, and processes.

## 8 HYBRID MODELING FOR CYBER SOCIAL LEARNING SYSTEMS (YILMAZ)

Advances in the theory and methodology of Cyber-Physical Systems (CPS) development have enabled connections between our physical infrastructures and computation at multiple scales and at all times. As we immerse these systems into our daily lives to provide radical improvements, the next frontier is expected to be the integration of CPS with socio-technical processes (Sullivan 2017). Such integration facilitates continuous improvement through mutual feedback between cyber and social systems, which constitute people, machines, computing, communities, organizations, and physical infrastructures (e.g., air traffic control, smart power grid). The resultant Cyber Social Learning System (CSLS) aims to improve the performance of human systems through advances in computational methods, design, social thinking, policy, norms, law, and governance. Such systems will involve not only human intensive, but also socially complex processes that provide services such as healthcare, education, transportation, and city services.

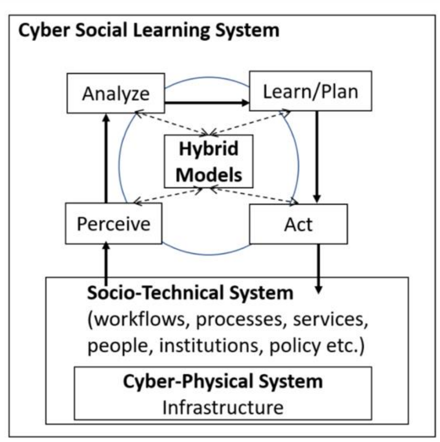


**Figure 4:** Cyber Social Learning Systems.

Both the physical and socio-technical domains, as shown in figure 4, involve open environments that include representational heterogeneity and significant uncertainty. That is, a CSLS spans many scales from individual to the dyad, group, sector, and society while adapting to achieve high fitness in an evolving environment. Computational models that aim to influence the governance and influence of such systems need to exhibit characteristics consistent with their heterogeneity as well as adaptive nature (Tolk 2014). In this position statement, I highlight the role of multi-models (Yilmaz and Ören 2004) in managing heterogeneity and in facilitating adaptation to deal with uncertainty, and stress the role of run-time hybrid models in providing a framework to support learning in CSLSs.

### 8.1 Implementing Hybrid Models as Multi-models

As highlighted in (Mustafiz et al. 2016), the development of CPS involves the development of hybrid models that encompass multiple levels of abstraction and different paradigms. Also, in a recent panel paper (Mustafee et al. 2017), hybrid modeling is construed as the process of merging two or more components of different categories to generate something new, combining the characteristics of these elements into something useful. Consistent with these definitions, multi-models (Yilmaz and Ören 2004; Yilmaz et al. 2007) provide a conceptual framework for implementing a broad range of hybrid model types. A multi-model is a modular model that subsumes various submodels, possibly with distinct formalisms and under different paradigms, which together constitute the behavior of a complex multi-stage, multi-aspect, and multi-resolution system. Awareness about the design space and types of multi-models, as delineated in (Yilmaz and Ören 2004), facilitates proper selection of model types to problems with matching characteristics. Moreover, the use of multi-models in the implementation of hybrid models promotes adoption of proven and effective design principles (Yilmaz et al. 2007) that bring systematic methodological support and a unified framework to engineer hybrid models. For example, a critical requirement for hybrid models for cyber social learning systems is the need for dynamic model updating (Yilmaz and Ören 2004) through continuous learning during both not only design, but also the deployment phase of a system.

### 8.2 Shifting the Focus from the Context of Justification to the Context of Discovery

Using hybrid models with distinct problem representations can change our perspective and expand our horizons in the way M&S studies are conducted. Hybrid models can foster creativity by enabling discovery of new strategies and policies in CSLS. There are many examples in the history of science about how exploring distinct problem representations can trigger creative leaps in understanding complex phenomena. For instance, at the end of the 18$^{th}$ century, a significant shift occurred from the theory of phlogiston of combustion to oxygen theory, enabled by a change in the representation of the problem. Chemical experiments on combustion resulted in the observation of (a) solid materials and residues and (b) heat, flame, and smoke produced during the combustion process. The latter explained the hypothesis of phlogiston, suggesting that phlogiston was driven out of materials during the process of combustion. However, advances in the measurement of the pressure and volume of gas molecules enabled scientists to observe that significant quantities of oxygen molecules were absorbed, and carbon dioxide molecules were produced. A shift in the focus of the representation of the combustion phenomena to gases as opposed to heat and flame changed our understanding of combustion and led to the emergence of the oxygen theory.

Similarly, in the domain of CSLS, the possibility for emergent behavior and the degree of contextual uncertainty requires an exploratory phase in the design of behavioral mechanisms. Such exploratory modeling with ensembles of models under a multi-modeling framework results in the discovery of robust solutions that can perform reasonably well across a wide range of possibly unforeseen situations, instead of exhibiting optimal behavior in a controlled and fixed environment. This shift in focus from the justification of an authoritative model to the context of discovery and iterative evaluation of increasingly accurate ensemble of models requires fostering a capacity of programmable abductive model building. Unlike deductive and inductive strategies that are prevalent in M&S studies, abductive reasoning starts with a portfolio of general behavioral mechanisms and then proceeds with evaluation to determine their efficacy and fitness to the environment. The discovery process is expected to take place in a simulated setting to facilitate training the system and to discern useful behavioral models across multiple aspects as well as levels of abstraction and resolution. An example of such simulated training of ensemble of multi-models is the Symbiotic Adaptive Multi-simulation approach (Mitchell and Yilmaz 2008), which enables the discovery of behavioral rules of models across multiple resolutions under simulated scenarios.

### 8.3 Continuous Learning with Run-time Hybrid Models

Due to the dynamic and evolving nature of CPS and cyber social learning systems, retainment during system deployment of hybrid models that evolved during simulated training is necessary. The use of hybrid models as run-time models contributes in two ways. First, simulation of the system faster than real-time can generate anticipatory states that help make decisions for tuning the system toward achieving desired objectives. Second, multi-models continue to evolve and adapt as a result of reinforcement based on the feedback received from observed system data. Model calibration and selection can take place at run-time because of learned model/state values.

## 9 DISCUSSION

The expert position papers compiled in this contribution address many different facets of challenges that need to be addressed when integrating simulation solutions as computational capabilities into CPS. We will choose the best solutions available and compose them in support of the CPS objective, in other words, we combine the different characteristics of these components into something more useful: hybrid simulation.

The necessity to agree on a unifying formalism to allow for conceptual composability to support collaborative ensembles is a common theme, but there is no agreement yet on how to accomplish this. If we can apply co-simulation approaches, develop a new hybrid simulation formalism, or focus more on meta- and multi-modeling approaches is topic of ongoing research, making CPS safer and easier to manage and to protect against cyber-attacks.

That contributions of the M&S domain can significantly benefit the CPS community was recognized by every expert on the panel. Although the terms used are often still different, the underlying ideas start to align, e.g., the approach to use concepts, specifications, and operations as categories of increasing specificity is well aligned with the definitions of M&S categories by Mustafee et al. (2017), using paradigms, methods, and solutions.

All experts on the panel agree that it is worthwhile to continue research in this direction and communicate it via publications of interest to the CPS community as well as the M&S community with the objective to grow together from current multidisciplinary approaches via the state of interdisciplinary contributions to truly transdisciplinary solutions.

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## AUTHOR BIOGRAPHIES

**ANDREAS TOLK** is Divisional Technology Integrator at the MITRE Corporation. He holds a Master and a PhD in Computer Science. He is a fellow of SCS and senior member of ACM and IEEE. His email is atolk@mitre.org.

**FERNANDO BARROS** is a professor at the University of Coimbra, Portugal. He holds a PhD in Electrical Engineering. His research interests include Theory of Modeling and Simulation, Hybrid simulation and time-varying topology systems. His email is barros@dei.uc.pt.

**ANDREA D'AMBROGIO** is associate professor of systems and software engineering at the University of Rome Tor Vergata (Italy). His research interests are in the fields of model-driven engineering, dependability engineering and distributed simulation. His email address is dambro@uniroma2.it.

**AKSHAY RAJHANS** is Senior Research Scientist at MathWorks. He has an M.S. in Electrical Engineering and a Ph.D. in Electrical and Computer Engineering. He is a member of ACM and IEEE. His email is Akshay.Rajhans@mathworks.com.

**PIETER J. MOSTERMAN** is Chief Research Scientist and Director of the Advanced Research and Technology Office at MathWorks. He has an M.S. in Electrical Engineering and a Ph.D. in Electrical and Computer Engineering. He is a member of SCS and IEEE. His email is pieter.mosterman@mathworks.com.

**SACHIN SHETTY** is an Associate Professor at the Virginia Modeling, Analysis and Simulation Center at Old Dominion University. He holds a Masters degree in Computer Science and a PhD in Modeling and Simulation. His email is sshetty@odu.edu.

**MAMADOU K. TRAORE** is Associate Professor at Université Clermont Auvergne (France) and Professor at the African University of Science and Technology (Nigeria). He holds a Master and a PhD in Computer Science. He is a fellow of SCS and member of ACM. His email is traore@isima.fr.

**HANS VANGHELUWE** is a professor at the University of Antwerp, Belgium and an Adjunct Professor at McGill University, Montreal, Canada. He is the chair of the EU COST Action IC1404 on Multi-Paradigm Modelling for Cyber-Physical Systems (MPM4CPS). His email is Hans.Vangheluwe@uantwerpen.be.

**LEVENT YILMAZ** is Professor of Computer Science and Software Engineering at Auburn University with a joint appointment in Industrial and Systems Engineering. He holds M.S. and Ph.D. degrees in Computer Science from Virginia Tech. His email is yilmaz@auburn.edu.

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