ABSTRACT

Socio-Cyber-Physical Systems are ubiquitous in today’s world. They are inherently complex systems built out of many large-scale systems that encompass different perspectives and numerous stakeholders. This leads to several challenges in managing their complexity and emergent behavior. In addition, these systems tend to include many adaptive and autonomous systems with different goals and different adaptations to environment changes or failures. The design, analysis, and testing of such systems is inherently challenging but is becoming critical due to their wide adoption. In this panel, we aim to discuss some of these challenges and potential solutions.

1 INTRODUCTION

Socio-cyber-physical systems (SCPS) are systems that integrate technological devices, software, and networked communications and operate in the physical world, also affecting the social environment (Calinescu et al. 2019). This integration offers incredible potential to SCPS to respond intelligently to actions and through their responsive and adaptive decision making processes. Examples include smart cities (Volkov 2018), healthcare (Dey et al. 2018), manufacturing (Frazzon et al. 2013) and agriculture (Rijswijk et al. 2021), and the integration of social, cyber and physical systems within these examples have outstanding potential to improve the quality of life of their users and the efficiency of their processes. Many challenges arise as SCPS expand in scale and complexity, including modeling and representation of such systems, their implementation, the integration of artificial intelligence models within traditional modeling and simulation, and verification and validation. In this panel, we focus on challenges arising from complexity and emergent behaviors, and from ensuring the resilience of such systems.

Complexity exists at many levels within a system, including structural, behavioral and knowledge levels, and emergent behavior is an expected consequence of complexity. However, to achieve resilience, it is critical that emergent behavior is understood, and, if its effects are negative, that it is mitigated (Davis 2005; Johnson 2006; Mogul 2006). As systems grow in the number and complexity of components, as well as the type of interactions and coupling between components, these emergent behaviors are becoming critical
to analyze (Johnson 2006; Mogul 2006; Bedau 1997; Holland 1999). In other cases, a reverse process is undertaken, where a specific system of systems is designed and implemented with the specific aim of it exhibiting an emergent behavior. Lastly, as SCPS grow in maturity and complexity, new systems are added to existing legacy systems. This poses challenges related to interoperability and composability at high levels (?), model representation, as well as resilience and robustness when newly components interact in unpredictable ways with legacy systems.

In recent years, advances in complexity theory and modeling and simulation has led to the analysis of a plethora of emergent properties examples, from flocks of birds, ant colonies, to the appearance of life and of traffic jams. In software systems, connection patterns have been observed in data extracted from social networks (Chi 2009) and trends often emerge in big data analytics (Fayyad and Uthurusamy 2002). More malign examples of emergent behavior include power supply variation in smart grids due to provider competition (Chan et al. 2010), the Ethernet capture effect in computer networks (Ramakrishnan and Yang 1994), and load-balancer failures in a multi-tiered distributed system (Mogul 2006). As emergent properties may have undesired and unpredictable consequences (Mogul 2006; Ramakrishnan and Yang 1994; Floyd and Jacobson 1993), systems that exhibit such behaviors become less credible and difficult to manage.

Emergent properties have been studied since the 1970s (Bedau 1997; Holland 1999; Cilliers 1998; Gardner 1970; Seth 2008), and a number of methods for their identification, classification, and analysis exist (Seth 2008; Chen et al. 2007; Kubik 2003; Szabo and Teo 2012a; Brown and Goodrich 2014). Existing methods are usually employed on simplified examples such as the flock of birds model, where only three flight rules are implemented, as opposed to the myriad rules that affect flocking in real life. Approaches to identifying emergent behaviors can be categorised as either attempting to identify emergence as it happens, without prior knowledge, or as using a definition of an emergent property and trying to identify its root causes. In the first type of approaches (Kubik 2003; Szabo and Teo 2012a) formal methods or meta-models calculated from composed model states are used. A key challenge remains how to identify variables or attributes that describe the system components, or the micro-level, and the system as a whole, or the macro-level, and the relationships and dependencies between these two levels. Once these are defined, emergence can be specified as the set difference between macro-level and the micro-level, however these levels are extremely difficult to capture and computationally expensive to calculate. This does not happen when using a definition of a known or observed emergent property with the aim of identifying its cause, in terms of the states of system components and their interaction (Seth 2008; Chen et al. 2007). A key issue in these works is that a prior observation of an emergent property is required, and that emergent properties need to be defined in such a way that the macro-level can be reduced or traced back to the micro-level.

In addition to these challenges, most approaches (Seth 2008; Chen et al. 2007; Kubik 2003; Brown and Goodrich 2014) are demonstrated using simple models such as flock of birds or predator-prey, which have limiting assumptions and constraints when applied to more complex systems. For example, most approaches do not consider mobile agents (Kubik 2003), assume unfeasible a priori specifications and definitions of emergent properties (Szabo and Teo 2012a), or do not scale beyond models with a small number of agents (Teo et al. 2013; Szabo et al. 2019). An exception is the defense and homeland security domain, where mobile agents are key when modeling combat missions, peace support operations, disaster relief efforts, or humanitarian logistics operations (Aros et al. 2021; Lovejoy et al. 2021; Lucas et al. 2007; van Steenbergen and Mes 2020; Yale et al. 2020). Some of the myriad of models of epidemic spread also rely on mobile agents, either at the micro-level to model the spread of disease through school, workplace, and social interactions (Andradóttir et al. 2011; Chan 2011; Maharaj and Kleczkowski 2012) or at the macro-level to model the spread via travel between different cities or countries (Ruan et al. 2015). In the multi-agent systems community, approaches focus more on the engineering of systems to exhibit beneficial emergent behavior and less on its identification (Bemon et al. 2002; Jacyno et al. 2009; Salazar et al. 2011). However, approaches that engineer emergent behavior do not ensure that no other side-effects occur as a consequence.
Resilience in SCPS refers to the system’s ability to continue to operate at acceptable levels of quality of service (QoS) even when the system is unexpectedly disturbed. Disturbances include cyber attacks in various forms, full or partial failures of composing systems, and network failures or attacks. To achieve resilience, it is critical for the SCPS to have modules that are able to detect disturbances, devise appropriate remedial actions, and execute them. This involves the integration of research advances in distributed fault-tolerant control, cybersecurity, human-machine teaming, the design and implementation of appropriate metrics to measure resilience (Szabo et al. 2020), ensuring that the SCPS is self-adaptive and self-organised, and system modeling and simulation (Bennaceur et al. 2019).

The ability of an SCPS to self-adapt with a high level of cognition is critical for the resilience of such systems (Szabo et al. 2020). Self-adaptation refers to the ability of a system to independently identify the need to adapt, plan an appropriate course of action and undertake changes to address the adaptation requirement. This may include reconfiguring systems, reallocating resources, establishing new links between systems and services, restarting systems and repurposing systems. Other examples of critical properties for resilient SCPS include self-configuring, healing, optimising and protecting (CHOP) properties (Kephart and Chess 2003; IBM 2006). A self-configuring system is one that is able to automatically reconfigure itself in response to changing environments. A self-healing system is able to discover, diagnose, and correct system malfunctions without disruption to its operating environment. A self-optimising system automatically monitors and tunes resources to optimally meet end-user or business requirements. Finally, a self-protecting system anticipates, detects, identifies and protects against threats to the system.

From a modeling and simulation perspective, it is critical that SCPS are modeled and simulated in such a way that the specific conditions in which these necessary properties are realised are well understood, and the many possible existing approaches are evaluated. To achieve this, it is necessary for appropriate resilience metrics to be designed and implemented, and for them to be evaluated in proper settings. This is where digital twins provide outstanding benefits as the simulation models are able to evolve with changes in the SCPS.

2 EMERGENT BEHAVIOR, SELF-ADAPTATION AND RESILIENCE IN SCPS (SZABO)

Emergent behavior should be an expected occurrence in SCPS ensuring that provisions for its management are part of the modeling and simulation (M&S) approach from the start. This includes among others the representation of the micro and macro levels and an understanding of their relationships and their side-effect. This is no easy feat in any complex system, and SCPS introduce significant challenges through the need to model social and physical systems and their many interactions.

In addition, the above challenges are exacerbated when artificial intelligence and machine learning models are integrated within the SCPS, as many challenges arise with the integration of AI/ML within simulation environments. Firstly, it is difficult to define internal behavior of decision making AI/ML modules. Secondly, the definition of micro and macro levels needs to consider AI/ML models and how these affect micro-macro interactions.

It is a challenging task to model SCPSs at sufficiently low levels of detail due to their inherent size, complexity, and non-linear interactions between components. To address this, multi-agent systems have been proposed in the past to model multiple across systems interactions. By creating models where emergence is an easily attainable product derived from agents interactions, users are relieved from having to model every aspect of the complex system under study. Multi-agent systems which have been designed to exhibit emergence are usually engineered to focus on self-organization and co-operation between agents. These systems generally rely on a system expert to identify the emergent behavior. For example, human societies and the myriad ways that emergent properties can arise are generally modeled using this approach in order to study aspects such as norm emergence. However, even for systems that have been engineered to exhibit emergence it is imperative to ensure that no side effects occur and that other undesired properties to not appear and this remains a fundamental challenge.
M&S approaches will be critical in addressing these problems but of course the use of M&S to analyse resilience and emergent behavior in SCPS brings significant research challenges, as summarised below:

- **Specification and representation** - one of the ways in which modeling and simulation is used within SCPS is to provide assurances about specific system properties. To achieve this, evaluation frameworks must be in place, however a broad evaluation framework that covers all systems within the SCPS might not be attainable at a low level of granularity. In addition, SCPS are inherently multi-disciplinary and as such within each system there might be different best evaluation practices. Instead, the evaluation frameworks must consider and integrate evaluations at different resolution levels depending on the evaluation norms within each discipline.

- **Providing assurance** - one of the roles that M&S plays in SCPS is that of providing answers to many "what-if" scenarios. These answers would then, ideally, inform policy makers. It is in this setting that the validation of SCPS models and simulations becomes critical. However, performing the validation of composed models is still an open research problem (Szabo and Teo 2013; Mittal 2013) that is further exacerbated by the presence of emergent behaviors. It is extremely challenging to validate an emergent behavior, as it is almost impossible, using traditional validation methods, to distinguish between invalid system outputs and the outputs generated by the emergent behavior itself (Szabo and Teo 2012b). This challenge is even further exacerbated when considering bias (Tolk 2017), and bias is bound to appear when considering unexpected system behaviors.

- **Multi criteria-multi domain decision making** - decision making within an SCPS requires the analysis of multiple criteria from different sources within what is inherently an interdisciplinary problem, capturing constraints across many domains. Decision making algorithms must also make reasonable predictions about the future, or at least the outcomes of specific actions. However, the modeling within certain domains might not allow for prediction with sufficient level of detail or accuracy, and as such decisions must be taken in the presence of incomplete information. In addition, as many systems are connected together through some form of information passing medium, the SCPS becomes vulnerable to communication failures and thus decision making modules must consider incomplete and stale information.

3 **STEERING COMPLEXITY: MODELING & SIMULATION & VISUALIZATION DECISION- MAKING PLATFORMS FOR SCPS (CASTRO)**

Socio-cyber-physical systems (SCPS) are by definition multi domain systems that call for interdisciplinary treatment. Complexity is usually present already in each of the three domains, requiring models that can account for emergent behavior where microscopic level entities interact yielding macroscopic level observables and structures, which in turn can feed back to the microscopic level. This makes it increasingly plausible that the interconnection of multiple complex subsystems in each domain creates interdependencies that result in a multi-layered complexity that is even more difficult to unravel.

An illustrative example can be found in major metropolitan areas, where the organization of urban transportation must adapt to evolving needs that are shaped by medium-term economic cycles. Local authorities rely on data sensing and edge-fog-cloud computing infrastructures to respond in near real-time to unpredictable short-term events, while simultaneously planning for long-term phenomena such as gentrification and a desired tendency to reducing greenhouse gas emissions.

Dynamics in areas such as business cycles, urban traffic, the Internet of Things, population growth and environmental pollution lend themselves to descriptions as complex systems in their own right. How do the well-known M&S concepts of modularity, multiscale, multiresolution and multidomain change when such submodels need to be interlinked?

To take a step forward, M&S techniques for SCPS often aim to steer the system, whether it is to move it from a current state to a more desirable one (goal seeking) or to keep it operating in the face of unpredictable disturbances (resilience). In both cases, the concept of planning to intervene in the system
becomes relevant, together with the idea of the level of satisfaction with the results (error control). This requires the use of robust control theory to find appropriate intervention trajectories that keep the system operating within acceptable bounds.

However, even with advanced multi-objective control and optimisation techniques, complex interdisciplinary systems make it very difficult for stakeholders from different domains to agree in advance on objectives (in the form of constraints or desired operating points). At this stage, SCPS become a central part of the so-called "wicked problems" (Lönngren and Van Poeck 2021): complex, ill-defined problems that are difficult to solve due to high levels of uncertainty, conflicting objectives and multiple stakeholders with different, yet legitimate, perspectives and interests.

M&S environments can play a key role by providing an M&S-centric decision-making platform presenting models of wicked problems that are transparent, interpretable and trustworthy, and that can be integrated into existing human workflows and decision-making processes. Borrowing from the concept of digital twins, groups of stakeholders could reach consensus on possible ways to steer an SCPS to desired zones of operation or, conversely, to prevent it from entering into undesired ones. This way, a simulation model can also act as a facilitator for developing a common language among disparate disciplines to reason about wicked problems and their underlying complex systems.

The following are examples of key M&S-related aspects that are challenged by resilience and complexity in SPCS:

- **Performance.** In order to meet the needs of participatory multi-stakeholder modeling simulations need to resolve in a near to immediate way providing a sense of reactivity similar to that of a gaming experience. This becomes hard to fulfill when systems include several submodels expressed as detailed ABMs, therefore requiring efficient parallel simulation capabilities.

- **Visualization.** A richer visual experience can boost a common interdisciplinary understanding of the complexities underpinning SCPS, and therefore need to offer multiple simultaneous views on an evolving system, with multiple synchronized views, covering both desired and undesired evolutions of a model behavior, associated to different types of interventions. This requires visualization facilities that are not traditional, possibly via combinations of virtual reality, extended reality and immersive experiences.

- **Composable expressiveness.** While there have been significant advances in the ability to combine different modeling paradigms and worldviews into a single hybrid simulation (e.g., system dynamics, ABM, cellular automata and complex networks), the way in which modellers express these systems is still highly dependent on the specific tool chosen to define the hybrid model. The challenge of SCPS is to allow a group of modellers to express dynamics using domain-specific languages (such as those used in economics, telecommunications or ecology, to name a few) in a transparent way, so that at later stages the translation into hybrid simulation frameworks can be automated, while keeping the expressiveness of the languages as close as possible to the discipline of each stakeholder.

- **AI-assisted exploration.** As we witness an innovation avalanche brought by AI technologies, the question arises how AI can support and enhance, rather than replace, M&S-centered planning and analysis. Explainable and interactive Machine Learning provides an opportunity to bring people (stakeholders, domain experts and modellers) together to conduct simulation-centred exercises in a context where AI algorithms are dynamically trained with the decisions made by humans while trying to steer the SPCS under study towards desired modes of operation (and to avoid undesired ones). In this way, at any given moment, a group of analysts can be presented with AI-generated alternatives that could not have been foreseen beforehand, while being in control of discarding unacceptable suggestions that may violate ethical principles (e.g., introducing solutions based on segregation or other forms of discrimination). Then this poses the challenge of how to integrate such Human-in-the-loop Machine Learning approach with simulation models of SCPS to deal with resilience in a context of complex dynamics.
4 TWINNING FOR RESILIENCE AND COMPLEXITY IN SOCIO-CYBER-PHYSICAL SYSTEMS (DENIL)

Cyber-physical systems serve humans and human societies. They are created with a specific goal and purpose in mind. However, different types of evolution occur in the system during the life cycle of the system. The source that initiates the evolution can come from four dimensions: (a) CPS-to-socio-evolution: introduction of systems evolves the view of humans and societies on the needs and structure of the community or society. This can lead to the introduction of other systems that might need to interact with the socio-cyber-physical system or the system’s evolution. We will not look at this type of evolution in the rest of this talk. (b) socio-to-CPS-evolution: Human, community or societal needs evolve and alter the system’s requirements. Requirements to the system can be added, removed, or changed. (c) Environment-to-CPS-evolution: This evolution is pressured from the operational domain of the system, where changes over time can occur, including interactions with other systems. (d) Internal evolution: the system itself can evolve because of, for example, wear and tear, replacement of components (with a similar but not the same type of component), etc. Note that systems can be looked at from the instance and type level (a definition of a set of systems). System evolution occurs at the instance and type level. Some of the evolutions at the instance level lead to system-type variants. Keeping the complexity of evolution under control is a critical challenge in the further adoption of SCPS.

One of the current technologies for society is the digital twin. Several definitions of a digital twin exist in the literature; as such, we will only state one: “A set of virtual information constructs that mimics the structure, context and behaviour of an individual/unique asset, or a group of assets, is dynamically updated with data from its asset throughout its life cycle and informs decisions that realise value” (AIAA Digital Engineering Integration Committee 2020). Applications include but are not limited to real-time monitoring, system optimisation, quality control and waste management (Barricelli et al. 2019; Huang et al. 2021). Digital twins are applied in all societal and industrial sectors like aeronautics, medical, smart city, and manufacturing. The twinning paradigm is not new: it is based on methods, techniques and architectures developed to maturity in the last decades in the modeling and simulation community (Paredis and Vangheluwe 2022). We look at the twinning paradigm to address socio-cyber-physical systems’ evolutionary complexity and resilience.

4.1 The twinning paradigm for dealing with the evolutionary complexity of socio-cyber physical systems.

To control the evolutionary complexity of SCPS, we need to detect changes in the system (source d) and the operational domain (source c). Both a twin of the SCPS itself and its environment are therefore necessary. These twins allow us to do:

Continual Validation: View the system’s operation as a continuous stream of experiments. With a subset of these experiments, the underlying models of the twin can continually be validated. Detecting changes and variants (both short-term and long-term) would mean that the twin is no longer valid for the system. More research into continual validation techniques are required (Lugaresi et al. 2022; Mertens and Denil 2021).

Continual Experimentation: Continual validation requires experimental data. However, in some cases, the correct data is available for proper validation (Feng et al. 2022; Mertens and Denil 2023). Experiments should be carried out in the real world to capture this data. These in-the-wild experiments require proper experimental design not to endanger the system’s mission and optimize the information content gained from the data of the experiment.

Variant Management: Once the different variants are detected, they must be organised. At the system definition level, we can define twins that keep track of the different variants of the system. Lessons can be learned from model-based systems engineering, where feature diagrams are often used to capture variants of
systems. Model management techniques are also required to organise the underlying models. Architectures, possibly distributed, of these twins-of-twins are required to allow for such variant management.

4.2 The twinning paradigm in support of the resilience of socio-cyber physical systems

Having a validated twin available allows for the execution of different services that help in the resilience of systems.

**Monitoring and logging:** Monitoring and logging of sensor information allow the twin to monitor the system and log events. Dedicated services can be created that detect adversarial events and conditions.

**Experimentation for recovery:** Validated twins of instances of SCPS help in recovery. Different (semi-) automated experiments are created to simulate different recovery scenarios to explore the recovery space of the system. The outcomes of these experiments can be compared for trade-offs and implemented in the actual system. Again, monitoring allows for follow-up and adaptation.

**Evolution of the system for preventing adversarial conditions:** The detection of the adversarial condition leads to informing other systems (and variants). It allows the creation of tolerance to the adversarial condition or event.

5 BEYOND SCPS MODELS TO INSIGHTS AND ACTIONS (SANCHEZ)

Author Neil Gaiman writes “The more accurate the map, the more it resembles the territory. The most accurate map possible would be the territory, and thus would be perfectly accurate and perfectly useless” (Gaiman 2011). This is an important concept to remember as we develop and continue to use and update simulation models, particularly in the SCPS domain. The ultimate goal of the simulation modeling process is not a simulation model itself, but its use as an aid to decision making for very complex problems. We mention this up front because modeling necessarily involves abstraction—as modelers in the SCPS domain, our success should be measured by how useful and informative our models are, rather than their complicatedness or complexity.

Those familiar with data farming know it to be a powerful approach that has led to massive breakthroughs in the breadth, depth, and timeliness of the insights that can be gained from simulation models. (Readers unfamiliar with data farming should see, e.g., Sanchez et al. (2021) for an overview.) Ideally, data farming is an integral part of the simulation study process—from model development, through verification and validation, through model exploration and assessment. Data farming enhances simulation studies by leveraging the power of efficient large-scale designed experiments, the computing cycles in high-performance clusters or clouds, and a broad set of data analytics, data mining, and data visualization methods. From its outset, data farming also recognized the importance of rapid model prototyping as part of a collaborative development process (NATO 2014).

Three potential goals that have been proposed for simulation experiments are (i) developing a basic understanding, (ii) finding robust decisions or policies, and (iii) comparing different alternatives (Sanchez and Sanchez 2017). These goals are more challenging in the complex setting of SCPS problems than for more focused problems such as factory layout or queueing system design—not just because of the complexity of the distinct domains and resulting emergent behavior, but also because of the large number of stakeholders with diverse backgrounds from different domains. I will focus on additional challenges for the first two goals, and finish with another long-term challenge.

- **Develop a shared understanding of SPCS models as a credible aids to decision making.** By understanding, we mean an understanding of the behavior between the model factors (often inputs or functions of inputs) to model outputs. We recognize there will generally be a the suite of models—some coupled more loosely than others. The large-scale experimentation that underlies the data farming approach facilitates answering “what if?” questions posed by stakeholders, and addressing larger questions such as “what matters most?” in an inferential (vs. observational) manner while exploring ways to influence the system. Establishing stakeholder credibility necessarily involves
them in the model development and assessment process. However, this is not easy. Bridging this credibility gap was recently identified as a major challenge for improving modeling and simulation-based support to major policy making (Castro et al. 2022). Here, model co-creation; interactive visualization; inherent flexibility to facilitate model updates and zoom in and out between micro-level and macro-level model components; and efficiency of the entire modeling-to-insight generation process were considered key areas meriting further research.

- **Find decisions or policies that are broadly accepted as robust or resilient.** As mentioned in earlier sections, models at different levels within different SCPS domains will use a variety of modeling paradigms at a variety of levels of fidelity. Those used to highly-detailed micro-level physical models must realize that micro- and macro-level socio models have value, and vice versa. The ‘detailed map’ quote above may help convey the value of different types and levels of modeling to a diverse group of stakeholders. A map of a subway system and a map of a country road network are both important and valuable—but for different decisions. Also, we in the simulation community are aware that in many cases, incorporating randomness into models may be more interpretable and computationally efficient than incorporating extensive levels of detail; this may assist in zooming in and out from macro- to micro-level models. In addition, data farming experiments can be applied to different domains and levels of the SPCS to identify ‘what matters?’ by answering questions such as ‘What are the most important outcomes to measure for the stakeholders most directly involved? What are the most impactful factors and interactions that affect these outcomes?’ In some instances, stakeholders may be more accepting of insights at other levels if they do not feel their concerns are being ignored. Experiments designed to detect whether input changes and uncertainties are amplified or dampened at higher levels, or whether higher-level outcomes are overly sensitive to variability and uncertainty at lower levels, might aid in discussions of robustness while reducing value judgments on the relative importance of different stakeholder domains.

- **Develop and promulgate a shared awareness of best practices.** Of course, this will not be all-encompassing; there is no ‘one size fits all’ approach. However, just as a shared understanding of a set of SCPS models problem develops over time, so a shared awareness among modeling and simulation professionals about approaches that work well (or not so well) for SPCS will improve our ability to help address these wicked problems. This may require intermediate steps as communities learn from one another.

In summary, although simulation support for seeking robustness, resilience, and other beneficial aspects of socio-cyber-physical systems is extremely challenging, it offers worthwhile and exciting opportunities.

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