

COMPLEX SYSTEMS MODELING AND ANALYSIS

Claudia Szabo¹

¹School of Computer and Mathematical Sciences
The University of Adelaide, Adelaide, AUSTRALIA

ABSTRACT

Undesired or unexpected properties are frequent as large-scale, complex systems with non-linear interactions are being designed and implemented to answer real-life scenarios. How to model the behaviors of entities in complex systems and their interactions, as well as how to analyze the large amounts of data generated in order to determine the effects of specific interactions or environmental changes remains an open problem. In this paper, we explore existing approaches to modeling complex systems. We present an in-depth overview of three properties exhibited by complex systems and present how they can be modelled in well known scenarios.

1 INTRODUCTION

Complex systems consist of numerous interconnected elements that interact with each other, often leading to emergent behavior that cannot be easily predicted by analyzing the individual components in isolation (Holland 2006; Mittal 2013; Özmen et al. 2013; Mittal 2013; Szabo and Teo 2013; Mittal et al. 2018; Manlio 2022). Examples of complex systems include social networks (Benham-Hutchins and Clancy 2010; Torres et al. 2021), robotics (Power and Berenson 2021), supply chains, healthcare networks (Birdsey et al. 2016), smart cities, the Internet of Things (Niazi 2013; North et al. 2013), and the Internet. In these systems, entities and their environments interact to achieve (usually desired) emergent properties. Complex systems are characterized by nonlinear dynamics, feedback loops, and sensitivity to initial conditions, which is further intensified when they are deployed in environments with frequent unexpected changes or contested resources (Honhaga and Szabo 2024; Manlio 2022).

Several critical properties of complex adaptive systems include self-organization, adaptability, and emergence. Self-organization occurs when entities interact to achieve some goal, or to move into a different collective state (Holland 2006; Mittal 2013; Dekkers 2015). Adaptability drives entities to a particular beneficial state (Walker et al. 2004; Chira et al. 2010; Mobus and Kalton 2015). The identification of system states where self-organization and adaptability occur is crucial to understanding complex system behavior and its causes.

Although research on emergent properties has been ongoing since the 1970s (Gardner 1970; Cilliers 1998; Holland 1999; Seth 2008), there are still very few methods their identification, classification, and analysis (Kubik 2003; Chen et al. 2007; Seth 2008; Szabo and Teo 2012; Brown and Goodrich 2014). Moreover, existing methods are typically applied to simplified examples that rarely occur in real life. For instance, the flocking model of birds suggests that flocks result from birds following three basic rules, whereas real-life flocking involves many more factors. Approaches to studying emergence can be broadly classified from two orthogonal perspectives. The first perspective focuses on identifying emergence as it happens, using formal or meta-models of calculated composed model states (Kubik 2003; Szabo and Teo 2012). A key challenge in this approach is identifying the variables or attributes that describe the system components at the *micro-level* and the system as a whole at the *macro-level*, as well as the relationships and

dependencies between these two levels. Defining emergence as the set difference between the macro-level and the micro-level is conceptually sound but difficult to capture and computationally expensive to calculate.

In contrast, the second perspective defines a known or observed emergent property and seeks to identify its cause in terms of the states and interactions of system components (Chen et al. 2007; Seth 2008). A key challenge with this *post-mortem approach* is that it requires a prior observation of an emergent property and necessitates defining emergent properties such that the macro-level phenomena can be traced back to the micro-level components. Current methods, often demonstrated using simple models like Flock of Birds or Predator-Prey, come with limiting assumptions and constraints when applied to more complex systems (Kubik 2003; Chen et al. 2007; Seth 2008; Brown and Goodrich 2014). For example, many approaches do not consider mobile agents (Kubik 2003), assume unrealistic a priori definitions of emergent properties (Szabo and Teo 2012), or fail to scale beyond models with a small number of agents (Teo et al. 2013; Szabo et al. 2019). In the multi-agent systems community, there is a greater focus on engineering systems to exhibit beneficial emergent behavior rather than on identifying emergent behavior (Bernon et al. 2002; Jacyno et al. 2009; Salazar et al. 2011). Additionally, methods that engineer emergent behavior do not always ensure the absence of unintended side effects (Szabo et al. 2009).

In this tutorial, we first present an overview of existing approaches that model and analyse complex systems. We then present an in-depth analysis of emergence, self-organization, criticality and adaptability and how these appear in two models. We also discuss how the modeling techniques could be used in more realistic systems.

2 MODELING AND ANALYSIS OF COMPLEX SYSTEMS

The literature on modeling and analysis of complex system is vast as complex systems are ubiquitous in a multitude of application domains and their study covers different perspectives (Sayama 2015; Bellomo et al. 2013; Tolk et al. 2018; Mittal et al. 2018; Holland 2014; Szabo and Birdsey 2017; Kossiakoff et al. 2020). We focus in this paper on how three relevant aspects of complex systems are modeled and analysed in the literature, namely, the *modeling paradigm and formalism*, the component or agent *interaction*, and *causation*.

2.1 Modeling Paradigms

Frequently used modeling paradigms include cellular automata, continuous field models, network topologies, and agent-based models. An automaton is a theoretical machine that changes its internal state based on inputs and its previous state. The state set is usually defined as finite and discrete, which often causes nonlinearity in the system's dynamics. Cellular automata (CA) (Ilachinski 2001; Wolfram 1983) are a set of automata arranged in a regular spatial grid whose states update simultaneously by a state-transition function that is applied uniformly. The state transition function includes references to the state of the cell's neighbours. The cellular automata is one of the first modeling formalisms used to describe the self-reproductive and evolvable behavior of living systems (Von Neumann and Burks 1966) and have since been used to model and analyse complex systems in a variety of domains including material science (Ogawa and Natsume 2021), chemical engineering, biology (Szabo et al. 2019), traffic analysis (Tian et al. 2021) and social and economical dynamics (Liu et al. 2021). A well-known example of a cellular automata is the Game of Life (Gardner 1970), which is discussed in more detail in Section 4.2.

The spatial and temporal dynamics within a complex system can be modeled and analysed using partial differential equations (PDEs), with early work including Turing's analysis of the chemical basis of morphogenesis (Turing 1990), which is an example of self-organization of complex systems. A simple first order representation of a PDE model is given below,

$$\frac{\partial f}{\partial t} = F\left(\frac{\partial f}{\partial x}, \frac{\partial^2 f}{\partial^2 x}, \dots, x, t\right) \quad (1)$$

with a note that the variable x is a point in a continuous space and that the state of the system $f(x,t)$ is defined over time and a continuous space. This approach is popular when there is a need to model spatial-temporal dynamics and a numerical simulation solution is feasible, with application domains such as biochemistry (Phan et al. 2024).

Network science has been widely used to study various complex systems in biology, ecology, sociology, economics, political science, management science, engineering, and medicine among others (Arney 2009; Börner et al. 2007; Barabási 2013). Starting with the seminal works on small-world and scale-free networks published in the late 1990s (Watts and Strogatz 1998; Barabási and Albert 1999) the perspective of modeling components of complex systems as nodes and their connections as links or edges has become very popular, with several important results stemming from this perspective.

Emergent behavior could be analysed using a graph representation of the complex system under study Gignoux et al. (2017), as a function connecting a micro state of the system to a macro state, as described in Section 3.1. In addition, several established advances from graph theory can be used for the analysis of complex systems when they are represented as networks, including connected components, min-max, Hamiltonian paths, graph and pathfinding algorithms. We refer the reader to extensive work by Harrison (2016) for further insight. Graph theory can also be used to demonstrate properties of complex systems and compute several relevant metrics. For example, the topological complexity of systems has been correlated with graph energy (Sinha et al. 2018; Pugliese and Nilchiani 2019; Nikiforov 2007). An example is the analysis of the resilience of a complex systems using graph theory, as proposed by Edwards et al. (2024). This approach builds on the approach proposed by Gao et al. (2016), who propose to model the complex system as a network, use a reduction of that network to a simpler model, and then measure that model's stability to various disruptions. Specifically, Gao et al. (2016) proposes a resilience index that measures the distance to tipping points. This mathematical approach is appealing as it is tractable, however the reductions to simpler models lose topological network information that could be useful in establishing hierarchies, or, as we saw in the approach by (Gignoux et al. 2017), to compute emergent behavior metrics. To address this, Edwards et al. (2024) propose to integrate this method with a measurement of a system's topological complexity using graph energy (Nikiforov 2007).

Agent-based models (ABMs) are the most generalized framework for modeling and simulation of complex systems, and have been used extensively in various application domains. The components present in a complex system can be modeled as agents that perform their respective actions and interactions (An et al. 2021). The modeling of these components as agents, allows for unnecessary information to be abstracted away leaving only the actions and interactions needed for a particular outcome. The agent-based models are then used in simulations to assist with research and analysis (Johnson 2006).

2.2 Causation and Interaction

The second perspective when modeling and analysing complex systems looks at causation, which captures the relationship between the macro-level and the micro-level entities in a hierarchical system (Holland 2006; Boi 2017; Foguelman et al. 2021). A frequent perspective used for analysis looks at the direction of the influence between the two, and classifies them as *upward* and *downward* causation respectively (Bitbol 2012).

Upward causation is the process by which the macro level entities or components influence or cause the macro level behaviors of the system. This implies that the emergence of a higher entity from a lower one is characterized by a certain causal process leading from the lower level entities to the higher level ones, so that the lower level can be seen as the cause and the higher level (Emmeche et al. 2000). *Downward causation* suggests that the higher-level entities can exert causal influence over the lower-level entities. More formally, (Emmeche et al. 2000), in a hierarchical system a given entity or process on a given level may causally inflict changes or effects on entities or processes on a lower level. For example, in neuroscience, the mind is considered a higher-level entity emerging from the complex interactions of neurons. Downward

causation would imply that mental states, such as beliefs or desires, can influence the behavior of individual neurons or neuronal networks.

The concept of downward causation challenges the traditional reductionist view in which all phenomena can be explained solely by understanding their constituent parts at the lowest level of analysis. Downward causation highlights the importance of emergent properties and system-level behaviors that cannot be fully explained by examining only the components of a system. An inherent challenge with this perspective is that it implies that the higher level entities have direct and immediate control on lower level entities, which contradict the law of physics. Nevertheless, Emmeche et al. (2000) suggest to reduce the strength of this influence by considering several levels of downward causation and the perspective where the macro level, through the environment, indirectly affects the micro level.

The *interaction* between entities in a system can be *direct*, in the form of the exchange of messages, data or knowledge, or *indirect*, where the exchange of information is either not immediate or happens through intermediaries or through the environment.

3 COMPLEX SYSTEMS PROPERTIES

A complex system can exhibit several important properties, that pose various challenges in their modeling and analysis. We discuss in the following emergent behavior, stability, criticality and adaptability.

3.1 Emergence

Emergence occurs when entities organize to behave collectively leading to the creation of an unpredictable *macro* state that cannot be decomposed into its *micro* components (Szabo and Teo 2013). However, some systems exhibit emergence without the presence of self-organization, such as a stationary gas (Mittal 2013). Emergence is present in many complex systems such as communities forming in social networks, formation of ant colonies, and rigid cellular structures (Chan 2011; Toole and Nallur 2014; Birdsey et al. 2015).

Bedau (1997) states that an emergent property can be defined as "a property of assemblage that could not be predicted by examining the components individually." Emergence can be seen in many real-world systems such as technological and nature-driven systems. For example, the neurons in the brain individually fire impulses but together form an emergent state of consciousness (Odell 2000). The flocking of birds is a well-known example of emergent behavior in nature. Independent birds aggregate around an invisible center and fly at the same speed for flock creation. The birds come together to create something that would be entirely indiscernible by studying only one or two birds. Two key examples of systems where emergent behavior is caused by interactions are the Flock of Birds model (Reynolds 1987), and the cellular automata Game of Life model (Gardner 1970). The former achieves its emergent properties through each bird flocking around a perceived flock center, while in the latter model the emergent properties are achieved by the patterns that are formed by the cells transitions between states. Studies that propose various processes of detecting and identifying emergent behavior mainly use either one or both of these systems to prove the validity of their proposed approach (Seth 2008; Chan et al. 2010; Chan 2011).

Multi-agent systems can be engineered to exhibit emergent properties (Fromm 2006; Savarimuthu et al. 2007). Several formalisms have been proposed to obtain or engineer emergent behavior, such as the DEVS extension proposed by (Mittal 2013; Birdsey et al. 2016), but they have yet to be employed in practice. 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 (Savarimuthu et al. 2007; Jacyno et al. 2009; Salazar et al. 2011). 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 (Savarimuthu et al. 2007; Jacyno et al. 2009).

Chan et al. (2010) highlight that agent-based simulation is the most suitable method for modeling systems containing unexpected or emergent behaviors, because it emphasizes that the actions and interactions between agents are the main causes for emergent behaviors. Several works support the use of agent-based modeling for studying emergent behaviors (Banks et al. 2000; Fromm 2006; Serugendo et al. 2006; Salazar et al. 2011; Pereira and Santos 2012). In addition to the Flock of Birds and Game of Life models, Chan et al. (2010) show that other complex systems such as social networks and electricity markets, implemented within an agent-based simulation, can exhibit emergent properties, which can then be identified. The methods in Chan et al. (2010) for detecting emergence rely upon the presence of a system expert, who can identify the emergent behavior.

Considerable research has been done in developing methods for the detection of emergence, and as discussed above existing methods assess emergence in either a *post-mortem* setting or a *live* setting (Szabo and Teo 2012). *Post-mortem* analysis methods are applied after the system under study has finished executing, and use data that was recorded during the execution (Szabo and Teo 2012). In contrast, *live* analysis methods are used while the system under study is executing (Chan 2011; Szabo and Teo 2012). Most existing works focus on *post-mortem* analysis methods (Chen et al. 2009; Tang and Mao 2014). In addition to *post-mortem* and *live* analysis, methods can be classified into three main types (Teo et al. 2013): *grammar-based* (Kubik 2003; Szabo and Teo 2013), *event-based* (Chen et al. 2007), or *variable-based* (Seth 2008; Szabo and Teo 2013; Tang and Mao 2014).

Some forms of *live* analysis involve *grammar-based methods*. These attempt to identify emergence in multi-agent systems by using two grammars, L_{WHOLE} and L_{PARTS} . Kubik (2003) defines that L_{WHOLE} describes the properties of the system as a whole and L_{PARTS} describes the properties obtained from the reunion of the parts, and in turn produces emergence as the difference between the two solutions. L_{WHOLE} and L_{PARTS} can be easily calculated as the sets of words that are constructed from the output of agent behavior descriptions. This method does not require a prior observation of the system in order to identify possible emergent properties or behaviors, which therefore makes it suitable for large-scale models where such observations are notoriously difficult (Teo et al. 2013). However, as grammars require a formation of *words*, the process through which these words are formalized can suffer badly as the model grows in scope, leading to computational issues, especially for large scale systems (Kubik 2003; Teo et al. 2013). To address this, some works attempt to identify *micro* level properties and model interaction, and performing reconstructability analysis on this data (Szabo and Teo 2013), however this analysis is required to take place in a *post-mortem* context.

Another example of a grammar based method is that proposed by Gignoux et al. (2017) who employ a graph theory perspective and define components as nodes in a graph/network, and their connection as edges. The micro level relationships are then derived as combinations of the influences of neighbours and local environment focal points. The macro level is defined as a hierarchical perspective on all components, and the question of whether an emergent behavior is present is reduced to whether there exists a function to transform from the micro state to the macro state. If that function does not exist, the system exhibits emergent behavior.

Some forms of *post-mortem* analysis involve *event-based methods*, in which behavior is defined as a series of both simple and complex events that changed the system state, as defined by (Chen et al. 2007). Complex events are defined as compositions of simple, atomic events where a simple event is a change in state of specific variables over some non-negative duration of time. These state changes, or state transitions, are also defined by a set of rules. Each emergent property is defined manually by a system expert as a complex event. It is the particular sequence of both complex and simple events in a system that lead to emergence occurring in the system. However, this method relies heavily on the system experts and their specific definitions. Furthermore, it can suffer from both agent and state space explosion making it unsuitable for large systems.

In *variable-based methods*, a specific variable or metric is chosen to describe emergence. Changes in the values of this variable signify the presence of emergent properties (Seth 2008). The center of mass of

a bird flock could be used as an example of emergence in bird flocking behavior, as shown in Seth (Seth 2008). Seth's approach uses Granger causality to establish the relationships between a macro-variable and micro-variables and proposes the metric of G-emergence, a near-*live* analysis method. This has the advantage of providing a process for emergence identification that is relatively easy to implement. However, the approach requires system expert knowledge as observations must be defined for each system. Szabo and Teo (2013) proposed the use of reconstructability analysis to determine which components interacted to cause a particular emergent property (defined through a set of variables). They identified the interactions that cause birds to flock (Reynolds 1987), the cells that cause the glider pattern in Conway's Game of Life (Gardner 1970), and the causes of traffic jams. However, their method is heavily dependent on the choice of the variable set that represents the micro and macro levels and requires the intervention of a system expert.

Variable-based methods from other fields, such as information theory and machine learning, have been adapted with the goal of emergence detection. Information theory approaches for detecting emergence have also been proposed by using such techniques as Shannon Entropy (Prokopenko et al. 2009; Gershenson and Fernández 2012; Tang and Mao 2014) and variety (Yaneer 2004; Holland 2007). These have advantages over other *variable-based methods* in that they can process large amounts of data efficiently. Tang and Mao (2014) propose measures of relative entropy that depend on the main emergent property of a system under study. However, these methods require the input of a system expert because they rely on the emergent property of a system being classified along with a specific function to be defined for that particular property. Machine learning classification techniques have also been proposed as a way of detecting emergence. A variant of Bayesian Classification (Brown and Goodrich 2014) has been used to successfully detect swarming and flocking behavior in biological systems such as the flock of birds model (Reynolds 1987). This approach involves identifying *key features* of an agent, such as how many neighbors an agent has, and uses this information to determine the likelihood that a random set of agents is exhibiting emergence. Other methods from machine learning have been utilized, such as Conditional Random Fields, and Hidden Markov Models in (Vail et al. 2007), but with the goal of activity recognition in domain specific contexts. Vail et al. used Conditional Random Fields and Hidden Markov Models somewhat successfully to determine if agents were performing a particular distinct action based on their relational position to other agents.

Another promising variable-based method is the Dynamic Cluster Index (Villani, Roli, Filisetti, Fiorucci, Poli, and Serra 2015), which measures the relevance of a subset of system variables to the emergence of system-wide behaviours. The DCI value is an information theoretical measure of how relevant a subset (S) of variables (k) is to the behaviour of the entire system (U). The first step in using the DCI method is to identify the subset sizes that will be analysed. The complexity of the calculations scales up quickly with large subset sizes. The second step is to generate the Candidate Relevant Subsets (CRSs) of system variables. These may be generated through random selection, or depending on the application they may be generated using a novel approach.

The third step is to evaluate the entropy of each CRS based on Equation 2, which determines the entropy of a single system variable x_i . This can be extended to determine the joint entropy of a set of system variables (see Equation 3 for the joint entropy calculation for a pair of system variables).

$$H(x_i) = - \sum_{v \in V_i} p(v) \log(p(v)) \quad (2)$$

$$H(x_i, x_j) = - \sum_{v \in V_i} \sum_{w \in V_j} p(v, w) \log(p(v, w)) \quad (3)$$

The resulting entropy values are used to determine two measures; the *integration (I)* and the *Mutual Information (MI)* of each CRS S . $I(S_k)$ measures the statistical independence of the k elements in S_k and is defined as:

$$I(S) = \sum_{x \in S} H(x) - H(s) \quad (4)$$

The Mutual Information $MI(S_k; U - S_k)$ is a measure of the mutual dependence between the CRS S_k and the rest of the system ($U - S_k$). The MI is defined as:

$$M(S; U - S) = H(S) + H(U - S) - H(S, U - S) \quad (5)$$

The results of the two measures are used in the Cluster Index calculation:

$$C(S) = \frac{I(S)}{M(S; U - S)} \quad (6)$$

If the MI calculation returns 0 this indicates two things; firstly, the value of DCI is not defined if $MI = 0$, and secondly this value may indicate a functional separation between the CRS and the rest of the system. As DCI values scale with subset sizes, a method to assess the statistical significance of the DCI of S_k is proposed through the use of a statistical significance index:

$$T_c(S_k) = \frac{DCI(S_k) - \langle DCI_h \rangle}{\sigma(DCI_h)} = \frac{vDCI - v\langle DCI_h \rangle}{v\sigma(DCI_h)} \quad (7)$$

where $\langle C_h \rangle$ and $\langle DCI_h \rangle$ represent (respectively) the average and standard deviation of the calculated DCI values for a particular subset size. v is the normalisation constant:

$$v = \langle MI_h \rangle / \langle I_h \rangle \quad (8)$$

Analyzing and determining how complex systems attain emergence can not only help system experts gain a deeper understanding of the system's behavior, but can allow them to configure them to encourage or discourage that particular form of emergence. The detection of emergence in complex systems has been performed significantly over the years (Szabo and Teo 2013; Birdsey and Szabo 2014; Toole and Nallur 2014). Szabo and Teo (2013) analyze emergence from a post-mortem perspective using reconstructability analysis. Birdsey and Szabo (2014) developed an architecture that requires a system expert to analyze snapshots of previous system executions and mark them if they exhibit emergence or not. These snapshots are then compared against when running the system, and various metrics are used to determine if the executing system exhibits emergence. Toole and Nallur (2014) proposed using correlation methods to detect downward causation while utilizing a decentralized approach. Szabo et al. (2019) proposed to apply this method on large scale flocks of birds models, with guarded success, mostly caused by the state space explosion of the calculation in the equations above.

3.2 Self-organization

Self-organizing systems are those that spontaneously reorganize after a disruption without any centralized control (Serugendo, Gleizes, and Karageorgos 2006). ? discuss how multi-agent systems can adapt to dynamic, heterogeneous environments through mechanisms inspired by natural systems such as ant colonies and flocks of birds. The mechanisms for integrating such behaviors are five fold, namely: (i) direct interactions between agents using basic principles such as broadcast and localisation; (ii) indirect interactions between agents and stigmergy; (iii) reinforcement of agent behaviours; (iv) cooperation behaviour of individual agents and (v) the use of a generic architecture.

3.3 Stability

Stability occurs when the system has reached some form of equilibrium (Miller and Page 2009; Chan 2011). Equilibrium is defined differently for each system, but can be characterized as either the system entering a stationary state, or a cycle. Systems that exhibit stability possess beneficial properties such as resilience and resistance (Mobus and Kalton 2015). In particular, resilience is a desired property as it allows a system to endure significant external input without major change, such as obstacles in the path of a large flock of birds, or large scale failures in a distributed system.

3.4 Criticality

Criticality is the single instance or sequence of time, before the system enters a stable, unstable, or emergent state (Ito and Gunji 1992; Miller and Page 2009). In many systems, criticality is observed at the edge of chaos or a bifurcation point (Mobus and Kalton 2015). Determining when entities are involved in self-organization or when self-organization has finished allows system experts to analyze its causes and design complex systems that encourage or discourage it.

3.5 Adaptability

Adaptability can be seen as either a precursor process to self-organization, e.g. adapting to a desirable state before self-organization can begin, or a sub-process, e.g. adapting to enhance current self-organization. Agents adapting allow the system to attain desirable states such as resilience and flexibility, and their adaptability can drive the system as a whole towards new states (Walker et al. 2004; Grisogono 2005; Miller and Page 2009).

4 EXPERIMENTAL MODELS

In this tutorial, we will look at the implementation of three models in NetLogo and NetworkX. We will analyse the emergent behavior exhibited by the models, as well as how they self-organize and adapt. We will also attempt to identify criticality. We present the three models below.

4.1 Flock of Birds

The Flock of Birds model (Reynolds 1987) captures the motion of bird flocking and is a seminal example in the study of emergence. At the macro level, a group of birds tends to form a flock. Flocks have aerodynamic advantages, obstacle avoidance capabilities and predator protection, regardless of the initial positions of the birds. At the micro level, each bird obeys three simple rules (Reynolds 1987):

1. Separation - steer to avoid crowding neighbors
2. Alignment - steer towards average heading of neighbors
3. Cohesion - steer towards average position of neighbors

We model this as a multi-agent system in which each bird is an agent that has the three movement rules defined above. Other bird attributes include initial position and initial velocities. In our experiments, the initial bird positions can be either fixed or assigned randomly at start up. Bird velocities are assigned randomly. The model parameters can also influence emergent behavior analysis. As such, we collect and analyze interaction graphs of Flock of Birds models with sizes of 20 and 50 birds, with fixed and randomly assigned position values, and randomly assigned velocity values.

4.2 Game of Life

Conway's Game of Life model (Gardner 1970) represents cells that interact with their neighbors to determine in what state they should be at the next time step, either alive or dead. At the macro level, patterns emerge between groups of cells, such as the Pulsar pattern as shown in Figure 1. At the micro level, the rules for each cell are as follows, where X , Y , and Z are the parameters for the Game of Life model (Gardner 1970; Chan et al. 2010):

1. A live cell with at least X and at most Y live neighbors will remain alive in the next time step
2. A dead cell with exactly Z live neighbors will become alive in the next time step
3. Otherwise, the cell will die in the next time step where $0 \leq X, Y, Z \leq \epsilon$ and $X \leq Y$, where ϵ is the maximum number of neighbors, which in a 2-dimensional configuration is 8

Certain combinations of X , Y and Z settings can reveal emergent behavior such as patterns, like the glider (Szabo and Teo 2013), and shapes appearing in the cellular structure (Chan et al. 2010).

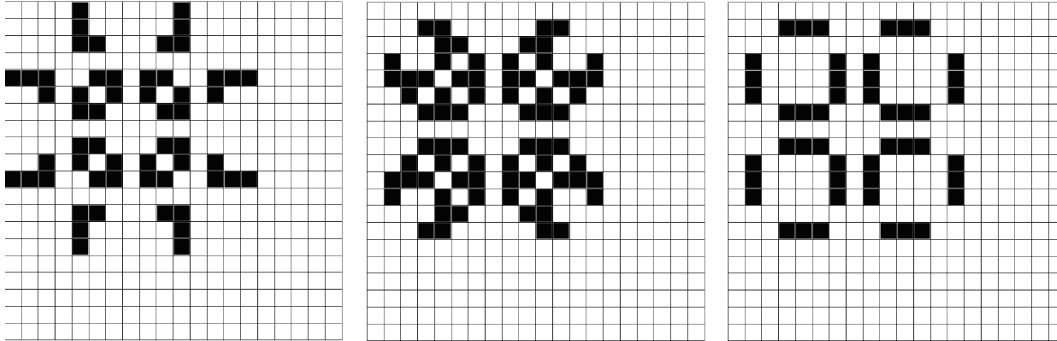


Figure 1: Game of Life with Pulsar pattern.

We model the Game of Life as a multi-agent system where each cell is an agent. A 2-dimensional grid of cells, of size $n \times n$, is established and the initial state of each cell is either fixed or chosen at random on start up. The attributes recorded for each cell are the cell state and the states of the cell's eight neighbors at the start of the time step. Snapshots are taken of Game of Life models with sizes of both 20×20 cells and 15×15 cells are collected and analyzed, each cell having a total of two possible states. Their initial states are either randomized or set to allow the creation of a particular pattern (Chan et al. 2010). For our experiments, we followed Conway's initial X , Y and Z rules, which are 2, 3, and 3 respectively.

4.3 Predator-Prey

The Predator-Prey model has been used in studying emergent behavior, with varying rule-sets (Chen et al. 2007). The Predator-Prey model has two types of agents, namely, Predators and Prey. As in nature, both types of agents wish to survive to create a new generation. Survival for the Predators is to eat whereas survival for the Prey is to avoid being eaten. The main difference of this model from the previous two is that agents can be added to or removed from the system during execution, and that the different agent types obey different rules. Specifically, Predators obey four rules while the Prey obeys two rules. The rules of the Predators are:

1. If a Prey is detected within distance d , kill the Prey with probability $p(predKill)$. If successful, the Prey is removed from the system immediately
2. If some Prey is killed, a new Predator is born at the Prey's location, after one time-step has passed
3. If a Predator is not within distance d , it dies with probability $p(predDeath)$
4. Move one step in any random direction if no Prey was killed and the Predator hasn't died

The rules of the Prey are:

1. Move one step in any random direction
2. Give birth to a new Prey at a random location with probability $p(preBirth)$

In our implementation, Predator and Prey are assigned initial random positions. Their velocities are also randomized at initialization as well as for each time step. The three rule probabilities, $predKill$, $predDeath$ and $preBirth$ are pre-defined. Both agent types have a common set of states, life and procreation, but the Predator has extra states to indicate if it has seen and/or killed some prey. If an agent is removed from the simulation, i.e. upon death, their life state is set to "dead". This is to ensure that no information generated by the system is lost as it may prove valuable to a particular metric.

5 MODELING OF COMPLEX ADAPTIVE SYSTEMS

This tutorial will first discuss the different definitions of emergence and their suitability for analysing different systems, from live or a-priori perspectives.

We will then look at the definition and implementation of different emergent behavior metrics within different stages of the simulation lifecycle. We will experiment with a flock of birds model, an ant model, a Game of Life model, and a Predator-Prey model and explore the use of interaction counts, DCI (Szabo et al. 2019) and Shannon information as emergent behavior metrics.

We will employ the NetLogo environment for the execution of these models and for the definition of the emergent behavior metrics, and discuss its advantages and disadvantages, in particular when considering the implementation of more complex metrics such as metrics for entropy or system complexity (?).

5.1 Game of Life

Consider the code for the Game of Life given in Listing 1. The questions we will be exploring during the tutorial will include when and how to compute emergent behavior metrics for this model.

Listing 1: Game of Life

```
to go
  ask patches
    [ set live-neighbors count neighbors with [living?] ]
  ;; Starting a new "ask_patches" here ensures that all the patches
  ;; finish executing the first ask before any of them start executing
  ;; the second ask. This keeps all the patches in synch with each other,
  ;; so the births and deaths at each generation all happen in lockstep.
  ask patches
    [ ifelse live-neighbors = 3
      [ cell-birth ]
      [ if live-neighbors != 2
        [ cell-death ] ] ]
  tick
end
```

5.2 Flocks of Birds

For the simple flock of birds model shown in Listing 2 (note: only flocking shown here), we will explore how to define, compute and visualise each of the metrics that are used to define the three complex systems properties defined above.

Listing 2: Flocks of Birds

```
to flock ;; turtle procedure
  find-flockmates
  if any? flockmates
    [ find-nearest-neighbor
      ifelse distance nearest-neighbor < minimum-separation
        [ separate ]
        [ align
          cohere ] ]
end
```

6 CONCLUSION

In this tutorial, we will discuss complex systems properties using three well-known models of Flocks of Birds, Predator-Prey and Game of Life. We will visualise the execution of these models in NetLogo and discuss how complex systems properties appear in other real-life systems. We will discuss how these properties can be modelled, considering issues of validation and accuracy. Lastly, the metrics used to determine whether an emergent property has appeared are critical for the validation of complex systems where these properties are inherently likely to appear. We discuss the implementation and suitability of a number of emergent behavior metrics.

REFERENCES

- An, L., V. Grimm, A. Sullivan, B. Turner, N. Malleon and A. Heppenstall. 2021. “Challenges, Tasks, and Opportunities in Modeling Agent-based Complex Systems”. *Ecological Modelling* 457:109685.
- Arney, C. 2009. “Linked: How Everything Is Connected To Everything Else and What It Means for Business, Science, and Everyday Life”. *Mathematics and Computer Education* 43(3):271.
- Banks, J., J. S. Carson, B. L. Nelson, and D. M. Nicol. 2000. *Discrete-Event System Simulation*. 3rd ed. Upper Saddle River, USA: Prentice-Hall, Inc.
- Barabási, A.-L. 2013. “Network Science”. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences* 371(1987):20120375.
- Barabási, A.-L. and R. Albert. 1999. “Emergence of Scaling in Random Networks”. *Science* 286(5439):509–512.
- Bedau, M. 1997. “Weak Emergence”. *Nous* 31(11):375–399.
- Bellomo, N., G. A. Marsan, and A. Tosin. 2013. *Complex Systems and Society: Modeling and Simulation*, Volume 2. Springer.
- Benham-Hutchins, M. and T. R. Clancy. 2010. “Social Networks as Embedded Complex Adaptive Systems”. *JONA: The Journal of Nursing Administration* 40(9):352–356.
- Bernon, C., M.-P. Gleizes, S. Peyruqueou, and G. Picard. 2002. “ADELFE: A Methodology for Adaptive Multi-agent Systems Engineering”. In *International Workshop on Engineering Societies in the Agents World*, 156–169. Berlin, Heidelberg: Springer.
- Birdsey, L. and C. Szabo. 2014. “An Architecture for Identifying Emergent Behavior in Multi-Agent Systems”. In *Proceedings of The 13th International Conference on Autonomous Agents and Multiagent Systems*, 1455 – 1456. New York, USA: Association for Computing Machinery, Inc.
- Birdsey, L., C. Szabo, and K. Falkner. 2016. “CASL: A Declarative Domain Specific Language for Modeling Complex Adaptive Systems”. In *Winter Simulation Conference*, 1241–1252 <https://doi.org/10.1109/WSC.2016.7822180>.
- Birdsey, L., C. Szabo, and Y. M. Teo. 2015. “Twitter Knows: Understanding the Emergence of Topics in Social Networks”. In *Proceedings of the Winter Simulation Conference*, 4009–4020 <https://doi.org/10.1109/WSC.2015.7408555>.
- Bitbol, M. 2012. “Downward Causation without Foundations”. *Synthese* 185(2):233–255.
- Boi, L. 2017. “The Interlacing of upward and Downward Causation in Complex Living Systems: On Interactions, Self-organization, Emergence and Wholeness”. In *Philosophical and Scientific Perspectives on Downward Causation*, 180–202. Routledge.
- Börner, K., S. Sanyal, and A. Vespignani. 2007. “Network Science”. *Annual Review of Information Science Technology* 41(1):537–607.
- Brown, D. S. and M. A. Goodrich. 2014. “Limited Bandwidth Recognition of Collective Behaviors in Bio-Inspired Swarms”. In *Proceedings of The 13th International Conference on Autonomous Agents and Multiagent Systems*, 405 – 412. New York, USA: Association for Computing Machinery, Inc.
- Chan, W., Y. S. Son, and C. M. Macal. 2010. “Simulation of Emergent Behavior and Differences Between Agent-Based Simulation and Discrete-Event Simulation”. In *Proceedings of the Winter Simulation Conference*, 135–150 <https://doi.org/10.1109/WSC.2010.5679168>.
- Chan, W. K. V. 2011. “Interaction Metric Of Emergent Behaviors In Agent-Based Simulation”. In *Proceedings of the Winter Simulation Conference*, 357–368 <https://doi.org/10.1109/WSC.2011.6147763>.
- Chen, C., S. B. Nagl, and C. D. Clack. 2007. “Specifying, Detecting and Analysing Emergent Behaviours in Multi-Level Agent-Based Simulations”. In *Proceedings of the Summer Computer Simulation Conference*, 969–976. New York, USA: Association for Computing Machinery, Inc.
- Chen, C.-C., S. B. Nagl, and C. D. Clack. 2009. “A Formalism for Multi-level Emergent Behaviours in Designed Component-based Systems and Agent-based Simulations”. In *From System Complexity to Emergent Properties*, 101–114. Berlin, Heidelberg: Springer.

- Chira, C., A. Gog, R. I. Lung, and D. Iclanzan. 2010. "Complex Systems And Cellular Automata Models in the Study of Complexity". *Studia Informatica Series* 55(4):33–49.
- Cilliers, P. 1998. *Complexity & Postmodernism*. Abingdon-on-Thames, UK: Routledge.
- Dekkers, R. 2015. "Complex Adaptive Systems". In *Applied Systems Theory*, edited by R. Dekkers, 169–190. Switzerland: Springer.
- Edwards, C. M., M. Vierlboeck, R. R. Nilchiani, and I. M. Miller. 2024. "Method for Measuring Resilience of Complex Systems Using Network Theory and Graph Energy". *IEEE Open Journal of Systems Engineering* 2:15–25.
- Emmeche, C., S. Køppe, and F. Stjernfelt. 2000. "Levels, Emergence, and Three Versions of Downward Causation". *Downward Causation. Minds, Bodies and Matter*:13–34.
- Foguelman, D., E. Lanzarotti, E. Ferreyra, and R. Castro. 2021. "Simulation of Emergence in Artificial Societies: A Practical Model-Based Approach with the Eb-DEVS Formalism". *arXiv preprint arXiv:2110.08170*.
- Fromm, J. 2006. "On Engineering and Emergence". *arXiv preprint nlin/0601002*.
- Gao, J., B. Barzel, and A.-L. Barabási. 2016. "Universal Resilience Patterns in Complex Networks". *Nature* 530(7590):307–312.
- Gardner, M. 1970. "The Fantastic Combinations of John Conway's New Solitaire Game 'Life'". *Scientific American* 223:120–123.
- Gershenson, C. and N. Fernández. 2012. "Complexity and Information: Measuring Emergence, Self-Organization, and Homeostasis at Multiple Scales". *Complexity* 18(2):29–44.
- Gignoux, J., G. Chérel, I. D. Davies, S. R. Flint and E. Lateltin. 2017. "Emergence and Complex Systems: The Contribution of Dynamic Graph Theory". *Ecological Complexity* 31:34–49.
- Grisogono, A.-M. 2005. "Co-Adaptation". In *Microelectronics, MEMS, and Nanotechnology*, 603903/1–603903/15. International Society for Optics and Photonics.
- Harrison, W. K. 2016. "The Role of Graph Theory in System of Systems Engineering". *IEEE Access* 4:1716–1742.
- Holland, J. 1999. *Emergence, From Chaos to Order*. Oxford, UK: Basic Books.
- Holland, J. H. 2006. "Studying Complex Adaptive Systems". *Journal of Systems Science and Complexity* 19(1):1–8.
- Holland, J. H. 2014. *Complexity: A Very Short Introduction*. OUP Oxford.
- Holland, O. T. 2007. "Taxonomy for the Modeling and Simulation of Emergent Behavior Systems". In *Proceedings of the 2007 Spring Simulation Multiconference*, 28–35. Piscataway, NJ, USA: Institute of Electrical and Electronics Engineers, Inc Press.
- Honhaga, I. and C. Szabo. 2024. "A Simulation and Experimentation Architecture for Resilient Cooperative Multiagent Reinforcement Learning Models Operating in Contested and Dynamic Environments". *SIMULATION*:00375497241232432.
- Ilachinski, A. 2001. *Cellular Automata: A Discrete Universe*. World Scientific Publishing Company.
- Ito, K. and Y. P. Gunji. 1992. "Self-Organization Toward Criticality In The Game Of Life". *BioSystems* 26(3):135–138.
- Jacyno, M., S. Bullock, M. Luck, and T. R. Payne. 2009. "Emergent Service Provisioning and Demand Estimation Through Self-organizing Agent Communities". In *Proceedings of the International Conference on Autonomous Agents and Multiagent Systems*, 481–488. New York, USA: Association for Computing Machinery, Inc.
- Johnson, C. W. 2006. "What are Emergent Properties and How Do They Affect the Engineering of Complex Systems?". *Reliability Engineering and System Safety* 12(1):1475–1481.
- Kossiakoff, A., S. M. Biemer, S. J. Seymour, and D. A. Flanigan. 2020. *Systems Engineering Principles and Practice*. John Wiley & Sons.
- Kubik, A. 2003. "Towards a Formalization of Emergence". *Journal of Artificial Life* 9(1):41–65.
- Liu, Y., M. Batty, S. Wang, and J. Corcoran. 2021. "Modelling Urban Change with Cellular Automata: Contemporary Issues and Future Research Directions". *Progress in Human Geography* 45(1):3–24.
- Manlio, A. O. 2022. "From the Origin of Life to Pandemics: Emergent Phenomena in Complex Systems". *Philosophical Transactions of the Royal Society A* 380(2227):20200410.
- Miller, J. H. and S. E. Page. 2009. *Complex Adaptive Systems: An Introduction To Computational Models Of Social Life*. Princeton, USA: Princeton University Press.
- Mittal, S. 2013. "Emergence in Stigmergic and Complex Adaptive Systems: A Formal Discrete Event Systems Perspective". *Cognitive Systems Research* 21(1):22–39.
- Mittal, S., S. Diallo, and A. Tolc. 2018. *Emergent Behavior in Complex Systems Engineering: a Modeling and Simulation Approach*. John Wiley & Sons.
- Mobus, G. E. and M. C. Kalton. 2015. *Principles of Systems Science*. NY, USA: Springer.
- Niazi, M. A. 2013. "Complex Adaptive Systems Modeling: A Multidisciplinary Roadmap". *Complex Adaptive Systems Modeling* 1(1):1–14.
- Nikiforov, V. 2007. "The Energy of Graphs and Matrices". *Journal of Mathematical Analysis and Applications* 326(2):1472–1475.
- North, M. J., N. T. Collier, J. Ozik, E. R. Tataru, C. M. Macal, M. Bragen *et al.* 2013. "Complex Adaptive Systems Modeling With Repast Symphony". *Complex Adaptive Systems Modeling* 1(1):15–23.
- Odell, J. 2000. "Agents and Emergence". *Journal of Object Oriented Programming* 12(9):34–36.

- Ogawa, J. and Y. Natsume. 2021. “Three-Dimensional Large-scale Grain Growth Simulation Using a Cellular Automaton Model”. *Computational Materials Science* 199:110729.
- Özmen, Ö., J. Smith, and L. Yilmaz. 2013. “An Agent-based Simulation Study Of A Complex Adaptive Collaboration Network”. In *Proceedings of the Winter Simulation Conference*, edited by R. Pasupathy, S.-H. Kim, and A. Tolk, 412–423. Piscataway, NJ, USA: Institute of Electrical and Electronics Engineers, Inc Press.
- Pereira, L. M. and F. C. Santos. 2012. “The Emergence of Commitments and Cooperation”. In *Proceedings of the 11th International Conference on Autonomous Agents and Multiagent Systems-Volume 1*, 559–566. New York, USA: Association for Computing Machinery, Inc.
- Phan, T. V., H. H. Mattingly, L. Vo, J. S. Marvin, L. L. Looger and T. Emonet. 2024. “Direct Measurement of Dynamic Attractant Gradients Reveals Breakdown of the Patlak–Keller–Segel Chemotaxis Model”. *Proceedings of the National Academy of Sciences* 121(3):e2309251121.
- Power, T. and D. Berenson. 2021. “Keep It Simple: Data-Efficient Learning for Controlling Complex Systems with Simple Models”. *IEEE Robotics and Automation Letters* 6(2):1184–1191.
- Prokopenko, M., F. Boschetti, and A. J. Ryan. 2009. “An Information-theoretic Primer of Complexity, Self-organization and Emergence”. *Complexity* 15:11–28.
- Pugliese, A. and R. Nilchiani. 2019. “Developing Spectral Structural Complexity Metrics”. *IEEE Systems Journal* 13(4):3619–3626.
- Reynolds, C. W. 1987. “Flocks, Herds and Schools: A Distributed Behavioral Model”. In *Proceedings of the 14th Annual Conference on Computer Graphics and Interactive Techniques*, SIGGRAPH '87, 25–34. New York, USA: ACM <https://doi.org/10.1145/37401.37406>.
- Salazar, N., J. A. Rodriguez-Aguilar, J. L. Arcos, A. Peleteiro and J. C. Burguillo-Rial. 2011. “Emerging Cooperation on Complex Networks”. In *Proceedings of the International Conference on Autonomous Agents and Multiagent Systems*, 669–676. New York, USA: Association for Computing Machinery, Inc.
- Savarimuthu, B., M. Purvis, S. Cranefield, and M. Purvis. 2007. “Mechanisms for Norm Emergence in Multiagent Societies”. In *Proceedings of the 6th International Joint Conference on Autonomous Agents and Multiagent Systems*, AAMAS '07, 173:1–173:3. New York, USA: Association for Computing Machinery, Inc <https://doi.org/10.1145/1329125.1329335>.
- Sayama, H. 2015. *Introduction to the Modeling and Analysis of Complex Systems*. Open SUNY Textbooks.
- Serugendo, G. D. M., M. P. Gleizes, and A. Karageorgos. 2006. “Self-Organisation and Emergence in MAS: An Overview”. *Informatica (Slovenia)* 30(1):45–54.
- Seth, A. K. 2008. “Measuring Emergence via Nonlinear Granger Causality”. In *Proceedings of the Eleventh International Conference on the Simulation and Synthesis of Living Systems*, 545–553. Piscataway, NJ, USA: Institute of Electrical and Electronics Engineers, Inc.
- Sinha, K., E. S. Suh, and O. de Weck. 2018. “Integrative Complexity: An Alternative Measure For System Modularity”. *Journal of Mechanical Design* 140(5):051101.
- Szabo, C. and L. Birdsey. 2017. “Validating emergent behavior in complex systems”. In *Advances in Modeling and Simulation: Seminal Research from 50 Years of Winter Simulation Conferences*, 47–62. Springer.
- Szabo, C., J. Groot, T. McAtee, and C. Pyromallis. 2019. “Who Did This: Identifying Causes of Emergent Behavior in Complex Systems”. In *2019 IEEE Symposium Series on Computational Intelligence (SSCI)*, 262–270. IEEE.
- Szabo, C. and Y. Teo. 2012. “An Integrated Approach for the Validation of Emergence in Component-based Simulation Models”. In *Proceedings of the Winter Simulation Conference*, 2412–2423.
- Szabo, C. and Y. M. Teo. 2013. “Post-mortem Analysis of Emergent Behavior in Complex Simulation Models”. In *Proceedings of the 2013 ACM SIGSIM Conference on Principles of Advanced Discrete Simulation*, 241–252. New York, USA: Association for Computing Machinery, Inc.
- Szabo, C., Y. M. Teo, and S. See. 2009. “A Time-Based Formalism for the Validation Of Semantic Composability”. In *Proceedings of the 2009 Winter Simulation Conference (WSC)*, 1411–1422. IEEE.
- Tang, M. and X. Mao. 2014. “Information Entropy-Based Metrics for Measuring Emergences in Artificial Societies”. *Entropy* 16(8):4583–4602 <https://doi.org/10.3390/e16084583>.
- Teo, Y. M., B. L. Luong, and C. Szabo. 2013. “Formalization of Emergence in Multi-Agent Systems”. In *Proceedings of the 2013 ACM SIGSIM Conference on Principles of Advanced Discrete Simulation*, 231–240. Montreal, Canada: ACM.
- Tian, J., C. Zhu, R. Jiang, and M. Treiber. 2021. “Review of the Cellular Automata Models for Reproducing Synchronized Traffic Flow”. *Transportmetrica A: Transport Science* 17(4):766–800.
- Tolk, A., S. Diallo, and S. Mittal. 2018. “Complex Systems Engineering and the Challenge of Emergence”. *Emergent Behavior in Complex Systems Engineering: A Modeling and Simulation Approach*:78–97.
- Toole, E. O. and V. Nallur. 2014. “Towards Decentralised Detection of Emergence in Complex Adaptive Systems”. In *International Conference on Self-Adaptive and Self-Organizing Systems*, 60–69.
- Torres, L., A. S. Blevins, D. Bassett, and T. Eliassi-Rad. 2021. “The Why, How, and When of Representations for Complex Systems”. *SIAM Review* 63(3):435–485.
- Turing, A. M. 1990. “The Chemical Basis of Morphogenesis”. *Bulletin of Mathematical Biology* 52:153–197.

- Vail, D. L., M. M. Veloso, and J. D. Lafferty. 2007. "Conditional Random Fields for Activity Recognition". In *Proceedings of the 6th International Joint Conference on Autonomous Agents and Multiagent Systems*, AAMAS '07, 235:1–235:8. Honolulu, Hawaii: Association for Computing Machinery, Inc.
- Villani, M., A. Roli, A. Filisetti, M. Fiorucci, I. Poli and R. Serra. 2015. "The Search for Candidate Relevant Subsets of Variables in Complex Systems". *Artificial Life* 21(4):412–431.
- Von Neumann, J. and A. W. Burks. 1966. "Theory of Self-reproducing Automata". *IEEE Transactions on Neural Networks* 5(1):3–14.
- Walker, B., C. S. Holling, S. R. Carpenter, and A. Kinzig. 2004. "Resilience, Adaptability and Transformability in Social–Ecological Systems". *Ecology and Society* 9(2):5–10.
- Watts, D. J. and S. H. Strogatz. 1998. "Collective Dynamics of 'Small-world' Networks". *Nature* 393(6684):440–442.
- Wolfram, S. 1983. "Statistical Mechanics of Cellular Automata". *Reviews of Modern Physics* 55(3):601.
- Yaneer, B.-Y. 2004. "A Mathematical Theory of Strong Emergence using Multiscale Variety". *Complexity* 9(6):15–24.

AUTHOR BIOGRAPHIES

CLAUDIA SZABO is an Associate Professor in the School of Computer Science at the University of Adelaide. Her research interests lie in the area of complex systems and on using simulation to identify and validate their emergent properties. Her email address is claudia.szabo@adelaide.edu.au.