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Cognitive Agent-based Computing-I

A Unified Framework for Modeling Complex Adaptive Systems Using Agent-based & Complex Network-based Methods



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This text is dedicated to sweet brother Super Zain

Muaz A. Niazi

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Acronyms

| CACOONS | Complex Adaptive COmmunicatiOn Networks and environmentS is a general term for large-scale communication networks which |
|---------|---|
| | exhibit some or all of complexity features of CAS |
| CAS | Complex Adaptive Systems |
| CNA | Complex Network Analysis is a domain-agnostic general term used |
| | for visualization, manipulation, generalization, and analysis of |
| | complex networks from the node, community as well as global |
| | perspectives |
| DREAM | DescRiptivE Agent-based Modeling entails building non-textual and quantitative descriptions of agent-based models |
| SNA | Social Network Analysis is analysis of the social infra-structure of communities often using CNA |
| VOMAS | Virtual Overlay MultiAgent System entails using a software engineering approach to build validated agent-based models |

Abstract

This set of SpringerBriefs introduces multidisciplinary researchers to a unified framework for the modeling and simulation of Complex Adaptive Systems (CAS). We call this framework *Cognitive Agent-based Computing* reflecting an evolution in thought from separate research lines of agent-based modeling and complex networks to a single set of framework levels. These levels in turn have been designed such that a specific level may be chosen by a researcher to suit suitable research goals for using modeling and simulation as a means for developing a deeper understanding of the CAS.

These two particular paradigms have been selected specifically after much deliberation and Scientometric analysis of citation data. Thus the selection criterion for these paradigms was the widespread acceptance and usage by a large and vibrant multidisciplinary research community spread across domains as diverse as from Biology to Ecology, from Social sciences to Music, Archeology, and Computer Sciences. These researchers use these paradigms to explore the inherent complexity and emergence in different types of CAS ranging from natural CAS (such as life and all things associated) to artificial CAS (such as exemplified by largescale communication networks).

However, what really ties these paradigms together is the word "Cognitive" because the goal of researchers for all these case studies is to develop "cognition" or "understanding" of different aspects of the CAS under study. The second part of the framework title is the phrase "Agent-based Computing" which is at the core of the modeling. The fact of the matter is that in each CAS, we always focus on the agents or individuals and their (often nonlinear) interactions with each other and with the environment. But while these agents are part of the real world at times, the goal of the framework is to assist in the development of computational models, whether using Agent-based (where the agents are modeled in a simulation) or Complex Network-based methods (in which case, agents are considered to be

Owing to a lack of a term for CAS nature in communication networks, we call such networks Complex Adaptive COmmunication Networks and environmentS or CACOONS.

connected in the form of a graph or network). The implications of combining these two agent-based paradigms are numerous. First, it has long been known implicitly that these two modeling paradigms are useful for modeling CAS. However, the two paradigms have evolved more or less independently even though they are complimentary in nature. Consolidating these two paradigms in a single framework allows researchers to understand both paradigms and select one or the other based on their particular needs.

The first of the several parts of Cognitive Agent-based Computing presents a unified picture of the entire framework in addition to serving as a gentle introduction to Agent-Based Modeling (ABM) and Complex Networks (CN) specifically with the goal of presenting concepts to a multidisciplinary audience. It is important to note here that our goal is not to redefine these well-established paradigms but rather to develop a framework that builds on, extends, and utilizes existing techniques from ABM and CN-based modeling approaches in the form of a one-stop framework for multidisciplinary CAS researchers. Each of the parts following the first part is self-contained and gives details of a particular framework level illustrated with the help of case study examples. Our goal in structuring this way is to allow researchers with different interests to read and use different framework levels based on their research intent, as explained in the first part.

Briefly, Part II is concerned with using interaction data of different CAS components (humans, genes, computer nodes, peers, societies, countries, research papers, etc.) to develop and analyze network topological features of a given CAS. While Part II is about complex networks, Part III is a about exploratory agentbased modeling, or in other words, it is about how most, if not all, typical ABM models are developed and explored for conducting feasibility studies for further research. Part IV presents a new paradigm; while there are text-based methods of describing ABMs such as the ODD protocol, we present a formal and non-textual way of describing ABMs by using CNs. In contrast to text-based methods, where the goal is human readability, the goal of DescRiptivE Agent-Based Modeling (DREAM) is to allow for improvements in terms of machine readability for better storage and a formal comparison of ABMs based on a converted CN from any ABM. Finally in Part V, we demonstrate how empirical validation can be extended and combined with Virtual Overlay Multiagent System (VOMAS) allowing for Validated ABM, a problem which has been quite difficult to solve for most ABM researchers. In short, in this set of SpringerBriefs, we not only give an overview of two key paradigms which are used by researchers from different CAS domains, but also combine and extend these paradigms to give a framework structured in the form of levels for selective usage in their respective research studies.

Chapter 1 Introduction

The title Cognitive Agent-based Computing reflects a unified framework combining two key modeling paradigms for developing cognition/understanding of a special type of systems namely the Complex Adaptive Systems (CAS). These two paradigms have been selected based on a detailed Scientometric analysis of journals listed in the Thomson Reuters database (Niazi and Hussain 2011a). It can be observed in literature that both Agent-based Modeling (ABM) as well as Complex Networks (CN) based modeling in their works on complexity. Among these Mitchell (2009), Agentbased modeling has proven to provide an effective set of tools for the modeling and simulation of different types of CAS. However, in the past decade, it can also be observed that an alternative set of tools and techniques in the area of computational modeling of CAS has emerged alongside. Whereas agent-based models are computer simulation models and dynamic in nature, these other tools and techniques, are collectively tied with the concepts and topological analysis, characterization as well as simulation of what may technically be termed as "complex networks". These are essentially graph-based structures developed using data from interactions of CAS components originating from and related to both natural as well as nature-inspired systems. While agent-based and complex network-based models can be located in literature ranging from Biological to Social Sciences and even Communication Networks, what is common between these two modeling paradigms is the fact that they are both used to model with the same type of goals of understanding a single type of systems i.e. CAS.

This set of SpringerBriefs has been structured for cross-disciplinary CAS researchers who are interested in using different types of models to develop an understanding of their CAS of interest. In other words, these briefs can be used both as a tutorial in development of agent-based and complex network-based models in addition to acting as a guiding framework for multi-disciplinary CAS studies reflecting the cognitive evolution of a unified framework for the modeling and simulation of CAS. Thus, the proposed framework extends upon existing ideas and paradigms and utilizes both agent-based and complex network-based modeling

paradigms. In other words, it gives an overview to multidisciplinary CAS researchers on how to go about developing computational models of CAS, regardless of whether the CAS of interest originates from the Life Sciences, Social Sciences or Computer Sciences.

The presented unified framework is structured in the form of *four* concrete levels beset with several example case studies for use by multidisciplinary researchers interested in developing an understanding of the CAS system under study. A suitable level can thus be selected by researchers on the basis of their cognitive goal and available resources for conducting a case study. Thus, if there is an availability of network interaction data, researchers can choose the first level of the framework concerned with developing complex network models. If the goal of the CAS researchers is to conduct feasibility studies, the most suitable level of the framework is the second level which is concerned with exploratory agent-based modeling. The third level of the framework is about developing descriptive agentbased models for conducting studies, which can be useful for quantitative and visual comparison of models and concepts irrespective of disciplinary boundaries. The fourth framework level is about validated agent-based modeling concerned with developing verified and validated agent-based models, such as for use by hardcore science researchers. Each framework level is described in detail using multidisciplinary case study examples ranging from information science, social science, ecology, computer and life Sciences.

1.1 About the Agent Concept

The word "agent" means a number of different things to different communities. In addition, at times, the word itself may not even be used as such in the case of communities of researchers where "agent" and "individual" are used for the same set of ideas. As such, while the definitions of agents may be numerous and based on a particular discipline of interest, the essence of an agent is essentially the same. It lies in the notion of "something or someone, which acts". Since the usage goal of the framework is cross-disciplinary, it is important to note that this notion should encompass all possible definitions of "agents" and "individuals". Thus if we were talking about economies, agents could be persons, countries, provinces and concepts. In addition, if we were talking about the ecology of a forest, agents could be species, forests, plants, animals, bacteria, fungi and so on. Likewise, in Life Sciences, agents could be tumor cells, blood cells, virus particles, genes, chromosomes and so on. Moreover, if the domain was Computer Sciences, agents could be software agents, robotic agents, sensor nodes, and peers in file sharing and so on. In other words, in this context, we will not focus on a domain-specific definition of agent and instead adhere to a general notion of an agent. In simple terms, an agent would be anything in a system, which may be considered and identified by experts in any discipline and sub-domain of interest as playing an important, individual, interactive and interesting role in the system leading to behavior which may be termed as intelligent, rational, cognitive or emergent. Agent may also be expected to contribute to a certain level to some significant aspect of the "big picture". The exact definition of what should be developed further as an agent and what should not be treated as one would also be limited by the scope of the research exercise as shall be discussed later in this set of briefs. Thus, at times, even though certain entities can be modeled as agents, for a particular exercise, it simply may not make sense to model them this way. As an example, if we were studying social interaction of people in a shopping mall, it would still be possible to model each person as made up of cells, muscles and tissues. However, it would not make sense to do that for several reasons. Firstly, doing so would make computational modeling extremely difficult. In other words, the growth in requirements of model complexity is not matched by the available computational power availability. Second, it would give rise to specifying unnecessary details in the model. Adding extra details may actually lower the quality of validity of the model due to the mechanism of multi-tasking (in the absence of massively parallel computers capable of exact and realistic simulations of agents and interactions).

To summarize, the skill of most appropriate agent definition for any given CAS requires experience and intuition acquired in the light of previous studies in literature. Another goal of this set of briefs is to serve as a starting point as well as a reference for examining how to develop concepts of agents in different models such as agent-based and network-based models by looking at existing examples of a variety of case studies across different disciplines developed throughout the different parts of the briefs.

1.2 A Framework for Complex Adaptive Systems

While there is general consensus in literature as to what systems might be CAS, one of the first definitions of CAS can be noted by Cowan and Feldman (1986).

"Systems comprising large numbers of coupled elements the properties of which are modifiable as a result of environmental interactions"

Examining literature, it appears that CAS may be more of a notion rather than a formal classification (Holland 1992; Miller and Page 2007; Mitchell 2009). In general CAS is considered as a special class of natural and artificial complex systems. Based on ideas originating from several disciplines ranging from the sciences and humanities, talking about CAS has a specific notion which is unlike the traditional concept of systems; CAS is a system where "The whole is more than the parts" and complex behaviors such as emergence can be observed. In other words, CAS are systems unlike other systems or even complex systems. The specific notion of system-wide adaptation and the nonlinear interactions of constituent components is perhaps what separates CAS from the general notion of complexity.¹

¹ Some researchers prefer to use the term complex systems (Mitchell 2009) in general while others adhere strictly to CAS (Miller and Page 2007).

CAS are made up of numerous and individually simple components which interact in a nonlinear fashion, thereby giving rise to global and, often, unanticipated, unprecedented and unpredictable behaviors. Phenomena and mechanisms associated with CAS include "emergence",² self-organization (Gershenson and Heylighen 2003) and self-assembly (Pelesko 2007). While an intelligent observer may be able to discern these phenomena at a higher levels of abstraction (Boschetti and Grav 2008), these phenomena are not easily quantifiable at the micro level. At times, while emergent patterns have been noted to be both interesting as well as unprecedented from the so-called "reductionist" point of view, it has been observed by CAS researchers that there is no known way of predicting these patterns based solely on an understanding of the individual components. Thus, an understanding of the individual components of a CAS is not enough to develop an understanding of the entire system (Kitano 2002) because it is the actual interactions of the components which plays a key role in the observed global behaviors. Taking a specific example, we can note that the human body is a CAS but our current understanding of the individual cells and biochemical involved at the micro level of the human body does not logically or formally lead to the concept of the actual capabilities of a human being. E.g. think, walk, move, read, educate etc.

With a strong presence and association with the natural sciences from the physical world, the notion of CAS is well-known to transgress disciplinary boundaries. Therefore, it is quite common to find researchers from different research domains developing various types of models of CAS. This phenomenon can be best noted by examining the results of search in relevant citation databases such as Google Scholar, Scopus and Web of Knowledge. These multidisciplinary researchers range from a wide and diverse set of disciplines in sciences and humanities such as social sciences (E.g. crowd behavior, effects of music on large populations etc.), ecological sciences (e.g. Emergence of particular species), economics (behavior and emergence of nations, self-organization in economies), system biology (Gene regulatory networks and other biological networks), archeology (inferring town formation from historical data) and others.

In spite of such a wide interest in CAS, it also can be noted that any detailed study of complex behavior can often turn out to be a non-trivial exercise; firstly because such a research study can involve a set of extensive data collection exercises which are used to develop models. Subsequently these models need to be correlated with these empirical results allowing for the development of an understanding of the underlying dynamics of the CAS.

Technically, developing an understanding of a CAS is associated with the formation of a special type of models called the "explicit" models. While "implicit" models are of a mental cognitive nature (Amadieu et al. 2011), "explicit" models (Epstein 2008) are perhaps more suitable for scientific

² According to the Oxford Dictionary, the earliest use of the term emergence dates back to 1755 by Brooke University "Beauty i. 10 From the deep thy [Venus'] bright emergence sprung." And formally defined as "The process of coming forth, issuing from concealment, obscurity, or confinement. lit. and fig. (Cf. emerge v. 3, 4.) Also said of the result of an evolutionary process".

communication amongst researchers. This difference is important because it is from an implicit model, that we create explicit models. However, the goal of these explicit models is to actually help in improving our implicit models.

In terms of effort and commitment, these models can range from exploratory, requiring a minor effort, to inquisitory, requiring perhaps man-years of effort and resources. These projects can also range from smaller to larger teams with different team structures of personnel for gathering real-world data and for developing agent-based or complex network-based models of various aspects of the system of interest. While CAS researchers conduct research in parallel disciplines and have an inherent interest in examining, comparing and contrasting models across disciplines, currently such comparisons are performed informally. As such, to the best of our knowledge, there is no unified framework for the multidisciplinary modeling and simulation of CAS. As such, most researchers resort to either performing informal comparisons (Mitchell 2009) or else evolving domain-specific methods of developing models (Grimm and Railsback 2005; North and Macal 2007; Gilbert and Troitzsch 2005; Lollini and Santo Motta 2006; Cioffi-Revilla 2011).

1.3 Modeling CAS

Epstein defines modeling as the development of a "simplified" representation of "something". Epstein also clarifies misconceptions about modeling and simulation giving a list of different reasons for modeling (Epstein 2008). He notes that modeling can be "implicit" (a mental model), in which case, "assumptions are hidden, internal consistency is untested, logical consequences and relation to data are unknown". Thus these types of models are not effective in the communication of ideas. The alternative is "explicit" models, which are more effective in communicating ideas and concepts associated with the model. In "explicit" models, the assumptions are carefully laid out and are coupled with details such as the outcomes of the modeling exercise. Another important feature of developing explicit models is that these models facilitate the replication of results obtained from the model by the scientific community.

For any CAS, the ability to come up with explicit models thus demonstrates the attainment of a level of understanding. Although CAS are extremely commonplace, they do not surrender themselves easily to modeling. In other words, while it is easy to make models of certain aspects of a CAS, it is quite difficult to model the entire CAS and its emergence. As such, in the absence of a single comprehensive framework governing various aspects of modeling and simulation of CAS, these systems have more or less been loosely modeled using a number of different paradigms with closely related roots. Previously, a number of aspects of CAS have traditionally been modeled by means of simplification of complex components to aggregates (Boccara 2010) such as by using differential equations, system dynamics or Monte Carlo simulations. However, more recently it can be noted by examining literature in Web of knowledge that CAS researchers often prefer the use of one of the two modeling approaches as follows:

- 1. Agent-based (or Individual-based) modeling approaches (Axelrod 1997).
- 2. Complex network-based approaches(Newman 2003).

To specifically comprehend the CAS modeling problem, a closer examination reveals that the development of a unified framework for modeling CAS would entail answering several open research questions. These questions, ordered from the less abstract to the more abstract, can be phrased as follows:

- 1. How to better develop models of the interaction data from various components of CAS?
- 2. How to describe CAS to facilitate communication across scientific and disciplinary boundaries?
- 3. In the case of a dearth of real-world data, how can CAS simulation models be validated primarily using meta-data or concepts?
- 4. In general, how can multidisciplinary CAS research projects be structured and executed based on an availability of resources and commitment?

Next, these four questions are examined in further detail.

1. Modeling interactions between CAS components.

As part of a search for suitable data for CAS modeling research, it is common to first discover that while there are a considerable number of existing data sources, not many of them might be useful for modeling. One key problem lies in the fact that most available data typically consists of statistical summarized data, which is often not very helpful in developing models of the exact nature of the underlying dynamics in CAS (Nations 2010). This approach does not give sufficient details to develop more advanced data-driven models. As such, CAS researchers need to figure out exactly how to structure their data collection exercise during their case study to be able to come up with models which actually give some useful information.

A particularly useful paradigm for developing models of interaction data is the Complex Networks Analysis (CNA) approach. Complex networks are essentially practical applications of the traditional graph theory (Bondy and Murty 1976). The idea is to use interactions and other relationships of various aspects and components in CAS to develop network models. Examples of these can include social networks with friendship relations forming links and individuals forming nodes or biological networks, where genes could be the nodes and co-expression could be links or wireless sensor networks, where links could be used to model reflect positioning of a device within the communication distance of another device and the nodes could each represent the sensor devices. Likewise, internet connectivity can be modeled as links with nodes being routers, gateways or countries.

Once the network models have been developed, CAS researchers can use network manipulation to extract useful quantitative as well as visual information about the topological structure of the system. Networks can be trimmed and particular types of nodes or links can be manipulated to highlight useful visual information about the topological aspects of the CAS. In addition, various quantitative measures such as network diameter, clustering coefficients, matching indices and various centrality measures such as eccentricity, betweenness, degree etc. can be calculated for the network. The basic idea behind this analysis is to find out important nodes or nodes which are unimportant. As an example, suppose there is a limited amount of a vaccine, then network analysis could allow you to discover the people with the highest degree centrality, in other words, nodes which are possible candidates for the vaccine. Thus, if we give vaccination to these nodes, they might help prevent the spread of the epidemic in the entire social network. Likewise, if we were to find out which gene was important in a set of genes, we could possibly use betweenness centrality to find its importance in terms of co-expression. Other than specific topological experimentation, it is also possible to classify a particular type of network (Such as either of small-World, Scale-Free or Random network models). Doing such an approximation also allows for the application of well-known properties of these networks to the studied network.

While there are numerous available software tools for developing complex network models, selecting the right type and quantity of data can pose to be a considerable challenge. Currently this is not an automatic process and thus existing data mining techniques cannot be directly applied to implicitly select important data from large number of data types and columns. Specifically CAS researchers may be looking for specific aspects of CAS tied closely with emergence and other complex phenomena. These concepts are cognitive in nature and are currently not easy to discern by means of purely computational techniques.

Taking a specific example of biological networks, currently a large amount of data sources are available in online repositories such as nucleic acid sequences and bioinformatics analysis clusters which can be used to execute complex algorithms. However, to actually develop networks, CAS researchers have to first understand and develop an implicit Mental model of exactly what should be a suitable node (e.g. a gene) and what would constitute a suitable link (e.g. co-expression) to ensure that the resulting network is useful for their domain. Some of these networks can themselves be quite complex and hierarchically structured. An example of these is the gene regulatory networks, which are themselves well-known as a system consisting of many sub-networks(Junker and Schreiber 2008). Other examples include protein interaction networks which are developed based on protein molecules in undirected graphs, signal transduction networks which are directed networks demonstrating various biochemical reactions and social networks such as friendship networks where the weighted links depend upon the perceived level of friendship of the subjects (persons) involved in the study (Nooy et al. 2005) etc. These concepts will be discussed in further details in this and subsequent parts, along with examples.

2. How to describe CAS to facilitate communication across scientific and disciplinary boundaries?

Researchers exploring CAS can come with a variety of different perspectives and disciplines. While they are experts in their subjects and can have significant domain knowledge, it is possible that they might not be comfortable with the nomenclature followed by other disciplines. As such, to describe CAS, there needs to be a common easily accessible description format which ties in closely with the CAS model but is not specific to a particular CAS scientific discipline. While it should not be highly technical, it should still allow the construction of descriptive models which should be comparable across case studies and disciplines. There are many inherent benefits of having such a description; firstly it would allow for a comparative study of CAS models across scientific disciplines and domains. Secondly, it would allow high fidelity of simulation models with the specification models. Thirdly, it can be used for learning CAS concepts from models of other domains. Networks include ontologies have previously been used to describe CAS. However, ontologies have not previously been used to describe CAS models in general and ABMs, in particular.

3. In the case of a dearth of real-world data, how can CAS simulation models be validated primarily using meta-data or concepts?

Being able to develop simulation models of CAS is one thing and being able to validate them is another. Unlike traditional simulation models, the concepts related to CAS are typically quite abstract in nature and not easy to describe verbally. While researchers have attempted to describe some aspects of a CAS, it has traditionally been quite difficult to give generalized definitions of CAS concepts such as emergence or self-organization etc. using terms globally acceptable by all disciplines. As such, the acceptability of the results of any CAS simulation model is tied closely with how valid these results appear to the researchers. While for social scientists, models might be considered valid if the results of a simulation appear similar to what they observe from population studies, for biologists, simulation models might need a much higher level of fidelity with the actual components of the system such as bio-chemical molecules etc. As an example, suppose a computational (in silico) model predicts that genes behave in a certain way. To test the validity of this model, it would require actual experimentation in the lab (in vitro) as well as perhaps in the actual organism itself (in vivo). As such, what might seem valid to scientists and researchers from one discipline might not be an acceptable validation for another set of scientists from another discipline. Thus, to have a comprehensive view of validation, it needs to be customizable across domains and projects. Currently developing validation can be a fairly nontrivial exercise and there is currently no way to structure the efforts of the Subject Matter Experts (SME) and the Simulation Specialists (SS). As such, validation of CAS simulation models varies from one case study to another without any basic common validation techniques unlike more traditional simulation models of complicated systems. Unlike most natural systems (e.g. Living beings) engineered systems are often better describable in terms of mathematical equations and mostly lend themselves better to generating suitable data for validation of models. This is not to say that mathematical models cannot be developed for natural CAS. The problem is that such models may not exactly and necessarily reflect the complexity of the interactions within the CAS. As an example, while there is a fairly standard mathematical model of an engineered system such as an artificial neural network representing more or less the complete aspects of the system, a typical mathematical model of a disease such as AIDS does not reflect the complexities or the social dynamics prevalent inside it. It may simply either reflect how the population is affected in general. Or else it may reflect how a viral load varies inside an individual. It would not be a dynamic model as is typically accessible using simulations.

Another problem associated with validation of CAS models is that at times, instead of being able to validate using data, the validation of complex concepts and emergent behavior of the CAS under study is required so as to ensure that the simulated system behaves close enough to the CAS being modeled. Such behavior is typically hard to put in an explicit model. Traditional validation techniques being typically data-driven either use various attributes from the results of a simulation model and compare them with "actual" results from the systems of interest or compare the results with another model. In the absence of either of these, SS need to rely on "Turing or face validation" (Balci 1998), where the observer compares output of the model visually based on previous experience with the system. In a CAS modeling scenario, at times, it can be difficult to acquire the exact data required for validation and thus, even though there might be some data, it might not always be a good candidate for traditional validation schemes. In other words, some points regarding validation of simulation models of CAS can be noted as follows:

(a) CAS are extremely interactive in nature. A simple change in the composition or interaction of components can massively change the global behavior. Being adaptive in nature, such type of changes however are quite the norm in a CAS. As such, any methods for validation which require comparison of plots as results might be misleading. Also, aggregate data in the form of purely statistical tables might not be a true representation of the actual CAS and might only represent a certain propagation of states of the CAS. The problem with CAS validation is that there might have considerably more complexity and emergence as might be apparent from observing only one aspect of the CAS. As an example, if we were to only focus on the complexity in the clotting, we might be unaware of the roles of different bio-chemicals and numerous cells from the immune system, which were also participating alongside the clotting reaction. Thus validation of the clotting would be just that. It would not validate the working of the entire CAS, which has a large number of emergent phenomena. In other words, this would like matching the color of a zoomed picture of a bird's yellow beak in a simulation with a yellow life jacket simply because the colors match even though the two are fundamentally different in every aspect except perhaps the color. Thus, even if "graphs" or "plots" appear to coincide, the actual models may be totally different and technically speaking, the validation would not be valid by itself.

- (b) Secondly, validation of CAS is tied closely with the interaction (run-time behavior) of the various "agents" inside the model and not just the output data. For a good CAS validation scheme, this important fact needs to be taken into consideration.
- 4. In general, how can multidisciplinary CAS research projects be structured and executed based on availability of resources and commitment?

CAS researchers develop models in a number of different ways and with many different objectives for different CAS aspects (Forrest and Jones 1994). The community of CAS researchers is firstly spread out in different disciplines and modeling paradigms. A common problem which is observed in modeling CAS is the lack of a formal approach to starting CAS studies. The development of a framework and toolset would expedite the piloting and further development of CAS models. It would also help structure concepts and assumptions in models by providing a common language for interdisciplinary research.

To the best of our knowledge, there is no existing multidisciplinary framework allowing the structuring of CAS case studies and model selection based on commitment levels or goals in addition to allowing a combination of complex network and agent-based modeling methods for multidisciplinary CAS researchers. Having such a single unified framework for multidisciplinary CAS research would thus assist considerably in developing and communicating CAS models across scientific disciplines and structuring CAS research projects.

1.4 Motivation

As noted in the previous section, there are several open questions associated with developing various types of "explicit" CAS models. The key problem here is the multidisciplinary nature of CAS systems. As such, there is neither a common methodology nor a set of concrete guidelines for developing CAS models spanning multiple scientific disciplines. Researchers can be unaware of exactly how to proceed and what to expect when developing CAS models. In addition, this problem is compounded by the fact that most CAS researchers are non-specialist in Computer Sciences and therefore in spite of being experts in their particular domains, they can tend to be neither interested in nor are often able to develop advanced highly technical models. However, it can be noted from an examination of multidisciplinary CAS literature that they still feel comfortable developing various types of explicit models with visual components (such as agent-based and complex network-based models).

This SpringerBrief has been motivated by this lack of a single unified framework for the modeling of complex adaptive systems. Although making models is a practice common to various types of CAS, CAS modeling has evolved vertically with little cross-flow of ideas between various application domains. As such, although there are numerous examples of applied modeling and simulation in literature, to the best of our knowledge, there does not exist a common guiding framework for interested multidisciplinary CAS researchers providing concrete guidance on how to approach CAS problems, how to develop different types of models and how to decide which type of data would be most suitable for developing models, how to describe simulation models with a high fidelity to the actual model, how to develop model descriptions allowing for visual and quantitative comparisons of models and last, but not the least, how to structure validation studies of CAS simulations. Such a framework might also assist in the removal of ambiguities in the usage of terms associated with CAS nomenclature³ prevalent due to a parallel evolution of modeling practices in different scientific disciplines, enabling different CAS models from different case studies and scientific disciplines to be comparable with each other.

1.5 Aims and Objectives

The aim of this research (proposed framework is introduced in Part 1 but case studies of individual framework in addition to other details of the levels are given in subsequent parts) is to work towards a set of unified framework guidelines allowing researchers interested in multidisciplinary and inter-disciplinary CAS studies to explore the development of explicit models of CAS by using a combination of complex network and agent-based modeling approaches based on their research goals and level of commitment.

1.6 Overview of the Briefs

Original research conducted and reported in this SpringerBrief is aimed at developing first steps towards a unified framework in the form of concrete guidelines coupled with detailed case study examples for use by multidisciplinary CAS researchers. Some of the key original contributions in the modeling and simulation of CAS are summarized as follows:

1. The key contribution is a unified framework allowing multidisciplinary researchers to plan their CAS research case studies formulated based on levels of research goals and commitment. The proposed framework uses a combination of

³ Examples include the terms individual-based modeling, agent-based modeling and multiagent systems. More details are given in Chaps. 2 and 3.

agent-based and complex network models to allow for interaction-based, exploratory, descriptive and validated models of CAS.

- 2. The proposed framework is structured in the form of different levels composed of a set of methodological guidelines. Each of the framework levels allows the planning and execution of a specific type of CAS research study based on the availability and type of data, the objectives of the case study and the expected levels of commitment.
- 3. The first two levels of the proposed framework are structured specifically to encompass existing modeling and simulation research which mainly uses complex network and agent-based simulation modeling techniques whereas the rest of the two framework levels allow for more advanced model development using a combination of these approaches.
- 4. The complex network modeling level of the proposed framework is structured and linked with the availability of suitable interaction data of CAS components. Therefore, it is only possible to develop complex networks when there is data related to CAS. If only aggregate or statistical data such as tables was available, it would not be sufficient to develop suitable networks. Data examples can be any form of interaction such as social interactions in a social network, expression of genes in a biological network, communication ranges of sensors in a sensor network or research papers citing other papers in a citation network. Using interaction data, complex network models can thus be developed for CAS exploration. These models can be manipulated and subsequently visualized using various mathematical and software tools giving qualitative as well as quantitative inference capability to the CAS researchers.
- 5. Using the exploratory agent-based modeling level, researchers can use agentbased modeling as an exploratory tool to develop proof-of-concept CAS models to explore feasibility of future research thus paving the way for more sophisticated techniques.
- 6. The descriptive agent-based modeling level of the proposed framework is useful for researchers who are primarily interested in cross-disciplinary communication and comparison of models. Descriptive modeling approach is being proposed which uses a combination of pseudocode-based specification and complex network modeling as a means of modeling ABM. There are several benefits of this approach; firstly it allows the description of CAS models in a way such that there is a high degree of fidelity of the model with the ABM. Secondly, it allows for quantitative, visual and non-code based comparison of CAS models developed in multiple disciplines. Thirdly, it allows the exploitation of learning opportunities for researchers by allowing the examination of models across scientific disciplines thus facilitating the creation of heterogeneous multi-domain ABMs.
- 7. The validated agent-based modeling level of the proposed framework is based on a step-by-step methodology for the development of in-simulation validation for agent-based models by means of an interactive collaborative effort involving both SME as well as the Simulation Specialists (SS). This approach is based on concepts from multiagent systems, software engineering and social

sciences. Using a systematic approach, the outcome of the methodology is an agent-based model of the CAS validated by means of design-by-contract invariants in the simulation model where the contract is enforced by means of in-simulation cooperative agents termed as the Virtual Overlay Multiagent System (VOMAS). Building a VOMAS allows SME and SS to collaboratively develop custom in-simulation verification and validation schemes for the CAS application case study.

8. The viability of the proposed framework is demonstrated with the help of various case studies spanning different individual scientific disciplines and some case studies spanning multiple scientific disciplines.

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Chapter 2 A Unified Framework

In this section, firstly an overview of the proposed framework is presented. Next the framework is described from two different perspectives firstly in terms of study objectives of conducting a CAS research case study and the expected level of commitment. Secondly, the framework is described in correlation with the availability and access to specific data types.

2.1 Overview of the Proposed Framework

For the sake of practicality, the framework guidelines have been developed in the form of levels of abstraction. Thus, CAS researchers can opt for modeling at a particular level depending on factors such as availability of data, meta-data as well as the level of interest and how much time CAS researchers can invest in pursuing a research project. In addition, example case studies are presented to demonstrate the usage of various framework levels. Based on the proposed framework, research in CAS can be conducted by choosing and subsequently following one of the following four proposed levels for developing CAS models:

• The complex network modeling level of the framework is useful if interaction data is readily available. In this level, complex network models of CAS can be developed using this interaction data and subsequently Complex Network Analysis (CNA) can be performed for network classification as well as determination of various global and local quantitative measures from the network for the extraction of useful information. Such information can give details of emergent behavior and patterns which would otherwise have not been evident using statistical or other more traditional mathematical methods. Numerous software tools are available which allow for an analysis of complex network models.

- The exploratory agent-based modeling level of the framework extends existing ideas of agent-based modeling prevalent in multidisciplinary literature which focus on the development of exploratory agent-based models of CAS to examine and extricate possible emergent trends in the CAS. Building exploratory models allows CAS researchers to develop experimental models which help lay foundation for further research. These proof-of-concept models also assist researchers in determining the feasibility of future research in the domain using the selected model design.
- While text-based descriptions of models exist, such as the ODD protocol, these descriptions have primarily been designed for the human user. There is need to develop discipline-independent numerical and formal descriptions of models. While the previous framework models reflected existing research in ABM and CNs, this framework level combines both ABMs with a non-textual description to give a descriptive model of a CAS. Developing models at the descriptive agent-based modeling level of the framework entails developing concrete Descriptive Agent-based Models (DREAM) by using a combination of pseudocode-based specification, a complex network model and a quantitative model "fingerprint" based on centrality measures of the agent-based model which are all associated closely with the ABM. The pseudocode-based specification is developed in the form of non-code template schemas and has several benefits; firstly it is close to an executable specification but is not tied with any single programming language thus allowing use by CAS researchers for developing agent-based models based on the specification using tools of their own liking. Secondly, this specific type of specification allows a one-to-one correspondence of ABM concepts with the descriptive model. Thirdly this specification allows communication and comparison of models in multidisciplinary studies by using visual as well as quantitative methods.
- In addition to developing descriptions of models, an important feature needed for a framework would be a scheme of validation which would also encompass previous validation techniques such as empirical validation while allowing for specifying validation specific to CAS. The validated agent-based modeling level of the proposed framework is concerned with developing verified and validated agent-based models. This level allows performing in-simulation verification and validation of the agent-based models using a Virtual Overlay Multiagent System (VOMAS) based on a cooperative set of agents inside the simulation allowing the verification and validation of the CAS model by means of design-by-contract invariants. These invariants are developed as a result of collaboration of the Subject Matter Expert (SME) and the Simulation Specialist (SS). In this level, concepts originating from software engineering, multiagent Systems and social sciences are all used in tandem to propose a systematic methodology for ABM verification and validation.

2.2 Proposed Framework Levels Formulated in Terms of CAS Study Objectives

In Fig. 2.1, it can be noted how different framework levels can be used by multidisciplinary CAS researchers to develop models based on their particular study objectives and expected outcomes.

If there is sufficient interaction data available then the CAS research study can proceed by using the complex network modeling level of the proposed framework. In this level, researchers first analyze the data columns, extract suitable data, develop complex network models and subsequently perform network manipulation and complex network analysis for the discovery of emergent patterns.

However, as is often the case, if such data is unavailable and the goal of the research study is to determine the feasibility of future research, then it might be possible to feasible to proceed in their research study by using the exploratory ABM level of the proposed framework.

These two framework levels essentially can also be used to encompass existing CAS research studies which have primarily used either complex network modeling and analysis or else agent-based modeling or both in their analyses.

If however, the goal of the research is to perform an inter-disciplinary comparative case study then the descriptive agent-based modeling level of the proposed framework allowing for developing a DREAM model can be chosen. This particular framework level has the benefit of allowing for inter-disciplinary model comparison, knowledge transfer and learning.

Finally, if the goal of the study is develop simulations with a high degree of correlation with real-world systems such as in the development of decision support systems, then the appropriate framework level for usage would be the validated agent-based modeling level based on the development of an in-simulation validation scheme using the VOMAS approach. This framework level is also more suitable for large-scale team oriented projects and requires adherence to team-oriented protocols with the goal of a verified and validated agent-based model of the CAS system under study.

2.3 Proposed Framework Levels Formulated in Relation to Available Data Types

In the previous section, an overview of the different framework levels in relation to the CAS research study objectives was presented. In this section, we shall describe the framework in terms of available data or knowledge related to the CAS. Thus while the previous figure allows CAS researchers to choose a suitable modeling level, here we discuss the specific type of knowledge and data needed to pursue specific types of studies. As we can note from Fig. 2.2, a descriptive specification of the CAS model can be developed based on the metadata or knowledge about the CAS.

2 A Unified Framework



Fig. 2.1 An overview of the decision-making process for choosing framework levels in relation to CAS research study objectives

An ABM can be developed either from this specification or directly from the knowledge of CAS. The ABM can be verified and validated using in-simulation validation (which has been developed as a result of extensive meetings between SMEs and SSs) that is performed by building a VOMAS model. By the help of invariant constraints enforced by the cooperative agents forming the VOMAS, the simulation



Fig. 2.2 A detailed overview of the framework

can be verified and validated using in-simulation methods. In addition, if interaction data is available for the development of network models, complex network models can be developed and CNA can be used to manipulate and analyze various structural topological features of the interactions using various information visualization-based and mathematical tools.

2.4 Overview of the Rest of the Parts

Here, first an overview of the different explored case studies is provided. This is followed by an overview of the chapters.

2.4.1 Overview of Case Studies

To ensure that the research was in line with the norms of various CAS, we have worked in tandem with teams of CAS researchers and domain experts from life sciences, social sciences and telecommunications. The following list gives details of some of the case studies discussed in this set of SpringerBriefs as a means of examples of the application of the proposed methods associated with various levels of framework along in correlation with the Briefs:

- The proposed framework level is applied on two different case studies in the domain of Scientometric data of agent-based computing and consumer electronics domains.
- A comprehensive case study on the use of unstructured search algorithms from the domain of P2P networks in the domain of "Cyber-physical systems" (Wayne 2009) by the development of an "Internet of things" (Ashton 2009) has been presented.
- A case study on the development of a heterogeneous ABM of sensing single-hop Wireless Sensor Network for sensing complex behaviors of flocking "boids" is presented.

• Three different case studies are presented. The first case study is in the domain of ecological modeling and models forest fire simulations. The second is in the domain of multi-hop Wireless Sensor Networks modeled in the form of a Quasi Unit Disk Graph (QUDG). The third case study is in the domain of simulation of the evolution of researchers on the basis of their Hirsch index.

2.4.2 Outline of the Briefs

Here we give an outline of the set of Springer Briefs:

- Part-1. This part presents background and related work. In addition an overview of the entire framework is presented.
- Part-2. This part presents complex network modeling level of the proposed framework. These methods are further applied to different domains such as Agent-based Computing and Consumer Electronics.
- Part-3. This part presents exploratory Agent-based modeling level of the proposed framework. As a demonstration of the proposed methods, a comprehensive exploratory agent-based model in the domain of Cyber-Physical Systems is developed demonstrating a combination of unstructured P2P search methods to locate content in static and mobile physical computing devices.
- Part-4. In this part, descriptive agent-based modeling level of the proposed framework is presented. Descriptive modeling entails the development of a DescRiptivE Agent-Based Modeling (DREAM) model by using a combination of a complex network model, a quantitative centrality-based fingerprint and a pseudocode-based specification model with a high degree of fidelity with the actual agent-based model. As a means of demonstration of the proposed framework level, the DREAM approach is applied in a comprehensive case study of a heterogeneous CAS ABM of a WSN observing a set of flocking "boids".
- Part-5. In this part, the validated agent-based modeling level of the proposed framework is proposed. The proposed methodology based a team-oriented approach of in-simulation validation is demonstrated using three different application case studies from three different scientific disciplines of ecology, telecommunications and social simulation allowing for a proof of concept of the generalized and broad applicability of the proposed methods.

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Chapter 3 Complex Adaptive Systems

Next, we give basic background and literature review of various concepts needed for the understanding of the framework.

3.1 Overview

We start by first giving an overview of CAS and their key characteristics. Next we give specific examples of CAS from natural and artificial systems. Subsequently we give an overview of modeling of CAS. Next, we give a review of agent-based modeling tools. This is followed by a review of verification and validation of simulation models. Finally an overview of different communication network simulators is presented.

3.2 Complex Adaptive Systems (CAS)

CAS are a special type of complex systems which arise due to nonlinear interactions of smaller components or agents (Mitchell 2009). While it is difficult to exactly define CAS, (Holland 1996) notes that:

Even though these complex systems differ in detail, the question of coherence under change is the central enigma for each. This common factor is so important that at the Santa Fe Institute we collect these systems under a common heading, referring to them as complex adaptive systems (CAS). This is more than terminology. It signals our intuition that general principles rule CAS behavior, principles that point to ways of solving the attendant problems

The modern approach of CAS has evolved from a series of attempts by researchers to develop a comprehensive and general understanding of the world around us. Our world is burgeoning with interactive entities. Most times, such interactions manifest themselves as change of some type either internal to the entities (change of internal state) or else external (change of external state or behavior). In other words, these entities adapt in networks of interactions spread nonlinearly across the entire system spatially as well as temporally (Girvan and Newman 2002).

In the science of complexity, it is the "small" and "numerous" that govern changes in the "large" and "few". The interaction of small (micro) and perhaps simple components gives rise to structures and behaviors, which are amazingly complex when observed from the macro perspective (Miller and Page 2007). Comprehension of the intricacies of these systems is so hard that it has lead to not just one but a set of theories based on different observations and different types of modeling methodologies targeting different aspects of the system.

A simple example of such systems is that of life. Although not easily quantifiable, living systems exhibit elegance absent in the monotonicity of complex but relatively inadaptable inorganic and chaotic systems. Life surrounds us and embosoms us. Every living system and life form known to us asserts itself with a display of a dualistic nature which on one hand is decrepit and frail and on the other it has its own tinge of sturdiness and resilience, hard to imagine in any engineered systems (Kaneko 2006). The frailty of complex living systems is apparent because all complex life forms seem stamped with a "certain" programmed expiration date because the growth and aging of most multi-cellular living organisms is governed by the complex behavior encoded in the genes. On the other hand, a closer examination reveals the Complexity and resilience working inside the systems. From apparent humble beginnings and small components (DNA, RNA, genomes, amino acids, proteins and cells etc.), the complexity of each life form emerges to give complex features such as muscles, tissues, systems, of which the most important is cognition and "self" for higher life forms.

A human embryo which starts as just a single cell replicates and forms a complete human being which is not just a blob of identical cells but has an extremely intricate and complex structure, with organs, systems and dynamics. Looking at the single cell embryo, it is hard to imagine how it could end up in forming this amazingly complex life form (Thomson et al. 1998).

If we examine the cell closely, it is hard not to think as to how exactly does this one cell, which divides into two and then four and so on, apparently suddenly bloom into complex structures without any apparent set of "physical" guiding forces or advanced sensory abilities such as one which coordinates all cells to form global structures. And when the structures do mature into systems, it makes one wonder how really do the multiple cells synchronize to gradually start the dynamic phenomenon associated with complex life forms, such as the blood flow, breathing, digestion, clotting, immune systems and emotions, thoughts, family, social systems and so on? The interesting part of all this is that the guiding principles of the entire life of the organism or life form are coded inside the genes, part of the cell's nucleus. Another example of similar complex systems is human and animal social systems, where interactions are once again the key to understanding the larger perspective of things. The concept of "country", "social or ethnic groups", "families", "clans", "universities", "civilizations", "religion" and so on are extremely powerful and govern the life of every human being. However, these phenomena are in one way or the other, rooted in the concepts of interactions. All this makes one thing very obvious. Our current science is known to miss the big picture of complexity. Developing this understanding further would assist us in understanding life, the universe and everything that exists (Miller and Page 2007).

This absence of the "complete picture" is at the heart of research in CAS and the closely related movements such as the "Complexity theory" (Mitchell 2009) and the "Systems Biology theory" (Kitano 2002). In contrast to reductionism which is rooted in simplifications and thus gives a misleading confidence that understanding the parts will somehow "ensure" that we will be able to understand the whole, the complex systems approach focuses instead on a specific meaning of the phrase "The whole is more than the parts". Here, literature notes that the key factor in understanding CAS is to understand the "interactions" of the parts which cannot be quantified easily.

3.2.1 The Seven Basics of CAS

Holland maintains that there are seven *basics* of CAS. Four of these are properties and three are mechanisms. These have been termed basics because he notes that other CAS-related ideas can be considered as derivates of these. The following discussion is based on Holland's description of properties and mechanisms of CAS (Holland 1996):

1. Aggregation (property)

The word "Aggregation" follows from "aggregate", which, according to the Oxford English Dictionary, means "Collected into one body". Aggregation is useful in two ways, firstly as a generalization where different items can be categorized in a single big and oft-reused umbrella, e.g. animals, plants, bags, baskets etc. In other words, this is a way of abstraction as well since it allows focus on the important details to be modeled and ignores those which can be ignored. This type of aggregation is perhaps classification and is more related to cognition rather than actual physical containment, to which the second type of aggregation may be attributed. Holland points out the formation of complex agents called meta-agents in living and social systems (whether natural or artificial) based on complex behavior of smaller, simpler agents.

An example can be seen in Fig. 3.1, where we notice that seemingly without any global intelligence, the shape of the melon is an example of emergence based on the complex interactions of its constituent components, such as skin, seeds and

Fig. 3.1 Peculiar shape and striations in a melon



other parts, which are made up of other structures, eventually coming down to cells and sub-cellular structures.

2. Tagging (Mechanism)

Tagging is a mechanism which is frequently observed in CAS. Tagging allows for the formation of aggregates. Tagging is exhibited in CAS in the same manner as flags are used to identify troops or messages are given IP addresses to reach the correct destination in a network etc.

3. Nonlinearity (Property)

Nonlinear interactions are the norm in CAS and are one of the reasons in the emergent global behaviors which indicate that the system is a CAS.

4. Flows (Property)

Another property of CAS is the formation of dynamic networks and flows. As such there are numerous attributes such as seen in Economics e.g. The Multiplier Effect when an extra amount of a resource is added to a flow causing it to transform as well as transmit between different nodes. Another important behavioral property that can be observed in flows is the recycling effect where resources are recycled over the flows via the network nodes thus enriching the emergent behavior. An example of the effects of recycling is the emergence of large number of insect and animal species in undisturbed forests as discussed by Nair (2007). Similar example is in the case of plants; Lowman notes the patterns of emergence, growth, mortality and herbivory of five rain-forest tree species (Lowman 1992).

5. Diversity (Property)

The species of a rainforest, people living in large towns, vendors in malls, structure of the mammalian brain all exhibit extreme diversity. So, it is rare to see the same type of components if any of these CAS are explored in depth.

Being a dynamic property, diversity also has self-repairing and self-healing characteristics. Disturbing the population of a particular predator in a forest can result in an increase of numbers of several prey species which can then result in an increase of numbers of the same or other predators. Lima (1998) notes that continuous predation can lead to major impact on entire ecosystems. Hein and Gillooly (2011) have recently demonstrated that dispersal and resource limitation can jointly regulate assembly dynamics of predators and preys.

6. Internal Models (Mechanism)

Internal models are a mechanism by which agents inside a CAS keep models of other individuals. On first looks, such a model would seem to be the property of only intelligent mammals. However, a closer look reveals that even the seemingly extremely simple life forms such as bacteria and viruses need to keep models of a certain kind of their environment and their hosts. These models are important for the survival of the species in general and thus the fact that a particular species still exists is a testimony that the species can defend its own in the particular environment (as has been happening for perhaps millions of years). Berg (2004) notes that E. coli exhibit model behavior because they exhibit motility towards regions in their environment that are deemed favorable.

7. Building Blocks (Mechanism)

Internal models as described in the previous section need to be enhanced by realistic mechanisms. These realistic mechanisms are termed as the "Building blocks". As an example, a diverse numbers of human beings form the 6 + Billion human population and they can each be basically differentiated from each other based on only a few set of building blocks such as eyes, nose, lips, hair, face etc. Variations in these blocks include changes in constituent attributes such as their color, shape etc. and eventually form the basis of the internal models.

In this section, we have noted how complex adaptive systems are structured and how they have a set of complex features which need to be examined closely to see why the systems behave in the peculiar manner at the global scale. We next talk a bit about "emergence".

3.2.2 Emergence

Emergent behavior in CAS has traditionally been considered difficult to define and hard to detect. Bar Yam (2004) defines emergence as follows:

Emergence refers to the existence or formation of collective behaviors—what parts of a system do together that they would not do alone

Yaneer also notes that emergence can be considered as a means of explaining collective behavior or properties of a group of components or agents or else it can

Fig. 3.2 Tree stem adapting structure temporally



also be used to describe a system in relation to the environment. Boschetti and Gray (2008) describe three levels of emergence:

- 1. Pattern Formation and detection such as oscillating reactions etc.
- 2. Intrinsic Emergence such as flocking behavior
- 3. Causal Emergence such as human behavior using messaging.

3.3 Examples of CAS

CAS can be both natural as well as artificial. Here we give some examples of different types of CAS. Next, we give specific examples of natural and artificial CAS.

3.3.1 Natural CAS Example 1: CAS in Plants

An example of adaptation in a natural system can be seen in Fig. 3.2 where we see a tree stem adapting according to the peculiar shape of an artificial metallic structure. One CAS which can be noted here is the complete plant. The plant itself is made up of numerous cells interacting and performing tasks based on programs from their genomes. However each cell is unaware of the large scale features of the plant or the way it interacts with the environment such as the emergent behavior of adaptation that can be observed in the figure in response to the position of the metallic structure as well as the path followed by sun for a better chance at getting sunlight. This emergent behavior can be seen as essentially a trait which has helped plants and animal species to survive over millions of years.

3.3.2 Natural CAS Example 2: CAS in Social Systems

While humans themselves are made up of several CAS originating from living cells and a variety of bacteria, viruses and other biochemical organic molecules. All these play an important role in the individual as well as social lives of living beings. An example is given here in the domain of the research process, which can, by far, be considered as one of the most complex social interaction, based on intelligent behavior.

A research paper published in a peer-reviewed venue represents the culmination of efforts of a large number of interactions. Some of the entities involved in a research paper are as follows:

- Authors and their Papers which were read during the study by the researcher
- Discussions and meetings with colleagues
- · Advice by advisors
- · Advice by conference or journal referees during the peer-review process
- And so on.

One way of understanding this all is to notice that this entire process reflects a highly dynamic CAS with multiple intelligent and inorganic (or even cyber-) entities such as papers, reviews and Journals. Several emergent behaviors can be observed here such as the propagation of research, formation of research groups, rise and fall of academic journals and their impact factors, emerging trends and these are all based on an enormous community of people spread globally, which do not even understand or even, at times, do not need to understand the exact structure and dynamics of how research leads to emergent behavior.

A quantitative study of scientific communication is technically termed as scientometrics (Leydesdorff 2001). Scientometrics requires the use of a multitude of sophisticated techniques including Citation Analysis, Social Network Analysis and other quantitative techniques for mapping and measurement of relationships and flows between people, groups, organizations, computers, research papers or any other knowledge-based entities.

Scientometrics sometimes involves the use of domain visualization, a relatively newer research front. The idea is to use information visualization to represent large amounts of data in research fronts (Chen et al. 2001). This allows the viewer to look at a large corpus and develop deeper insights based on a high level view of the map (Card et al. 1999). Visualization using various network modeling tools has been performed considerably for social network analysis of citation and other complex networks (White and McCain 1998). Various types of Scientometric analyses have previously been performed for domains such as HIV/AIDS (Pouris and Pouris 2010), Scientometrics, Mexican Astronomers, scientific collaborations (Barabási et al. 2002) and engineers in South Africa (Sooryamoorthy 2010). Extensive work on research policy has been performed by Leydesdroff (Leydesdorff 2001). Some of the recent studies in this direction include visualization of the HCI domain

(Chen 2006), identification of the proximity clusters in dentistry research (Sandström and Sandström 2007), visualization of the pervasive computing domain (Zhao and Wang 2010), visualization of international innovation Journals (Chun-juan et al. 2010) as well as identification of trends in the Consumer Electronics Domain (Niazi and Hussain 2011b).

Scientometric studies which combine co-citation analysis with visualizations greatly enhance the utility of the study. They allow the readers to quickly delve into the deeper aspects of the analysis. Co-citation analysis measures the proximity of documents in various scientific categories and domain. These analyses include primarily the author and the journal co-citation analyses. Journal co-citation analysis identifies the role of the key journals in a scientific domain. In contrast, the author co-citation analysis (White and Griffith 1981) especially by using visualization (White and McCain 1998) offers a view of the structures inside a domain. The idea is based on the hypothesis that the higher the frequency of co-citation of two authors, the stronger the scientific relation between them. Whereas document co-citation maps co-citations of individual documents (Small 1973; Small and Griffith 1974; Griffith et al. 1974), author co-citation focuses on body of literature of individual authors. In addition, co-citation cluster analysis of documents is useful for the display of the examination of scientific knowledge evolution structure at the macro level. In initial cluster analysis, techniques involved clustering highly cited documents using clustering based on single-links. Subsequently clustering is also performed on the resultant clusters numerous times (Small 1993). Recent techniques involve the use of computational algorithms to perform this clustering. These clusters are then color coded to reflect that.

If we were to take some of these entities, and analyze the data, we can come up with quite interesting networks e.g. as shown in Fig. 3.3. This network represents top papers, in terms of citations, with topics related to "agent-based modeling" from the years 1990–2010. As can be seen here, the network visualization is clearly allowing the separation of the top journals in this field in terms of "centrality" measures such as degree, betweenness, eccentricity or indices or clustering coefficients as described in previous section. Complex Network are not only formed from social interactions. Rather they can be developed from any CAS system interaction such as systems inside living beings (Junker and Schreiber 2008).

Journal Citation Reports (JCR) has been considered in literature as the key indicator of a Journal's scientific repute (Garfield 2000). It is pertinent to note here that previously researchers such as (Amin and Mabe 2003) have critically reviewed the way Journal impact factor might be used by authors and journals. While alternatively other researchers have proposed new alternative impact factors such as by Braun et al. (2007) and Fersht (2009). However, the fact remains that, in general, the scientific contributions listed in Thomson Reuters Web of Science are considered highly authentic by the overall scientific community (Garfield 2006; Moed et al. 1996).

Fig. 3.3 Complex Network model showing different Journals publishing articles related to agent-based modeling. Bigger caption represents a higher centrality measure explained later in the part



3.3.3 Artificial CAS Example 1: Complex Adaptive Communication Networks

In this section, we introduce complex adaptive communication networks. Complex adaptive communication networks are a recent advancement in artificial CAS. Primarily these are communication networks which have a large number of components resulting in behavior associated with CAS. These networks arise due to a recent rapid advancements in communication technology because today's communication networks such as those formed by wireless sensor, ad-hoc, Peer-Peer (P2P), multiagent, nano-Communication and mobile robot communication networks, are all expected to grow larger and more complex than ever previously anticipated. Thus, these networks, at times, can possibly give rise to complex global behaviors similar to natural CAS. As a result, network designers can expect to observe unprecedented emergent patterns. Such patterns can be important to understand since, at times, they can have considerable effect on various aspects in a communication network such as unanticipated traffic congestion, unprecedented increase in communication cost or perhaps a complete network/grid shutdown as a result of emergent behavior. Some well-known examples include the emergence of cascading faults in Message Queue-based financial transactions after New Year holidays(Niazi et al. 2006), recent cascading failures reported in the Amazon.com cloud(Gunawi et al. 2011), effects of viral and worm infections in large networks, effects of torrent and other complex traffic in Internet Service Providers and corporate networks, multi-player gaming and other similar P2P traffic in company intranets, self-organization and self-assembly related effects in sensor and robotic networks (Dressler 2007).

The torrent protocol is an example of an artificial CAS since it exhibits a number of interesting properties associated with CAS. It relies on software called the "torrent clients" which, as can be seen in Fig. 3.4 allow autonomous and almost anonymous interaction with other clients around the globe. The different



Fig. 3.4 Artificial global CAS formed by P2P clients observed using utorrent software

peers autonomously self-organize and adapt to both download as well as upload files. Here, the emergent phenomenon is the downloading of the file. The interactions, allocations of bandwidth, uploading and downloading of chunks are part of the nonlinear interactions.

The way this entire process the process of uploading and downloading (sharing) files works is outlined by Cohen in (2003) as follows:

- 1. The peer computer which starts to share a file breaks the file into a number of identically sized pieces with byte sizes of a power of 2 anywhere from 32 KB to 16 MB each. Each piece is hashed using SHA-1 hash function and this information is recorded in the. torrent file.
- 2. Peers with a complete file copy are called seeders and those providing the initial copy are called the initial seeders.
- 3. The torrent is a collective set of information about the file coupled with the information about tracker servers allowing peer discovery of downloaders.
- 4. The trackers give random lists of peers to other peers.
- 5. The different peers automatically self-adapt to download the complete file from distributed chunks of file from all over the globe.
- 6. Peers who only download and do not upload are punished by lesser bandwidth while peers who upload as well are given higher bandwidths.
- 7. The emergent behaviors here include the file sharing (upload and download) and reduction of peers who only download.

3.3.4 Artificial CAS Example 2: Simulation of Flocking Boids

In 1986, a computational model of flocking animal motion was presented by Reynolds (1987) called the "boids". The model is based on three separate but simple rules. The first rule is "separation" which involves steering to avoid crowding. The second rule is "alignment", which steers the boid towards the average heading of local flockmates. And the third rule is "cohesion", which steers towards the average position of local flockmates. The "boids" model has been considered a model of realistic simulations ranging from SIGGRAPH presentations to Hollywood. This model offers an example of complex adaptive behavior based on apparently local rules of the mobile agents or boids.

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Chapter 4 Modeling CAS

The word "Model" is defined by Merriam-Webster in 13 different ways:

- 1. obsolete: a set of plans for a building
- 2. dialect British: copy, image
- 3. structural design *a home on the model of an old farmhouse*
- 4. a usually miniature representation of something; also: a pattern of something to be made
- 5. an example for imitation or emulation
- 6. a person or thing that serves as a pattern for an artist; especially: one who poses for an artist
- 7. Archetype
- 8. an organism whose appearance a mimic imitates
- 9. one who is employed to display clothes or other merchandise: Mannequin
- 10a. a type or design of clothing b : a type or design of product (as a car)
- 11. a description or analogy used to help visualize something (as an atom) that cannot be directly observed
- 12. a system of postulates, data, and inferences presented as a mathematical description of an entity or state of affairs
- 13. Version

Critically speaking, modeling a system is important for the survival of the human race. The entire concept of cognition appears to be based on modeling. We start our learning by experiencing this world, which leads us to the development of cognitive "mental" models. Then we use these models to associate with other experiences or knowledge to keep learning. As an example a baby develops a first implicit "model" of heat if s/he touches a hot bottle of milk. Later on, in her life, she keeps learning more and more about temperature and heat while whether she consciously realizes it or not, all new models are rooted essentially with the basic cognitive model. This kind of models have been termed as "implicit" models (Fischbein et al. 1985).

Implicit models, however, are hard to express and are not very communicable. What one person perceives of a certain concept, might mean a totally different thing to another. This is the reason for the development of what Epstein, an authority in modeling, mentions as "explicit models" (Epstein 2008).

Modeling implies a certain level of understanding and prowess over the system and requires a deep study of certain aspects of the system. When it is not just one system, rather a group of systems, modeling implies developing abstractions, which can cover different domains.

Previous techniques have included focus on physics as a means of modeling. Such formal models typically are simplified models representing the system as e.g. Differential equations. Obviously by limiting an entire system to only a few equations implies that most aspects of the system including the components have been reduced to simple numbers, e.g. quantities such as change of numbers etc. However, more recently modeling CAS often entails using one of two basic methods of developing computational models i.e. either use of Agent based modeling to develop simulation models or else development of complex network models for analysis of interactions using real world or simulation data as shall be discussed in detail in the next section. Although these models prevail in literature, to the best of our knowledge, there is no unified framework, which outlines this set of ideas and couples them along with agent-based models.

4.1 Agent-based Modeling and Agent-based Computing

Agent-based Computing ranges from building intelligent agents to multiagent systems and agent-based simulation models. There has been considerable focus in the Artificial Intelligence and other research communities on something which has been termed agent-based computing (Wooldridge 1998; Jennings 1999). Although prevalent across a number of domains, there is considerable confusion in the literature regarding clearly a differentiation between its various flavors. Here we shall attempt to disambiguate its various levels by providing a hopefully clear set of definitions of the various terms and their uses.

4.1.1 Agent-oriented Programming

The first of the agent-oriented paradigm which we see is focused more on the increased use of artificially intelligent agents such as proposed by Norvig (2003). The focus here is on developing more complexity in an individual agent rather than on a large set of agents.

4.1.2 Multi-agent Oriented Programming

While agent-oriented programming focused on individual agents, it was difficult to actually design, implement and run multiple agents with such intricate internals because of the need for massively parallel computational resources for even simple problems. However, multiagent-oriented programming typically attempts to add at least some intelligence to agents and observe their interactions. One thing to note here is that typically such models have either few agents with a focus on certain aspects only, or else do not implement a whole lot of complex behaviors (Norvig 2003; Panait and Luke 2005a, b). The primary reason for not implementing all intelligent paradigms is the inability to perform all such calculations in real-time in any currently known artificial computational system. That is one reason why online algorithms in AI typically use simplistic mechanisms for searching such as heuristic functions other than purely reactive simple or table-driven agents (which can just perform an if else type of actions). Another key problem is the knowledgeengineering bottleneck (James 2007), where the agents had difficulty communicating with each other. Although partially solved by languages such as Knowledge Ouery Manipulation Language (KOML) (Finin et al. 1994) and DARPA Agent Markup Language (DAML) (Hendler and McGuinness 2000) and DAML + OIL (Connolly et al. 2007) language released in 2000–2001 time frame, practically large-scale intelligent agents have not seen the daylight of most commercial or real-life scenarios (such as earlier predicted by agent-technology evangelists).

4.1.3 Agent-based or Massively Multiagent Modeling

One particular application of agents, which actually has found extensive use is what is termed as individual or agent-based models. The key idea in these models is the focus on use of "simple" simulated agents interacting with a large population of other agents with emphasis on observing the global behavior. Here instead of the individual agents themselves, the interest of researchers is on the use of the interaction at the micro-level to observe features at the global values. The focus of main-stream agent-based modeling and simulation has been either social systems (Gilbert and Troitzsch 2005; Quera et al. 2010) or else ecosystems(Grimm et al. 2006; Railsback and Grimm 2011).

In this section, we shall review these paradigms further. Agent-based models (Bankes 2002) (or individual-based models as termed in some scientific disciplines) have been used for the modeling of a wide variety of complex systems (Bonabeau 2002). Their use ranges from as diverse as Biological Systems (Devillers et al. 2008; Dancik et al. 2010; Folcik et al. 2007; Galvao and Miranda 2010; Galvao et al. 2008; Guo et al. 2008; Huang et al. 2007; Itakura et al. 2010; Kiran et al. 2008; Lao and Kamei 2008; Bailey et al. 2009; Carpenter and Sattenspiel 2009; Rubin et al. 2008; Odell and Foe 2008; Robinson et al. 2008;

Santoni et al. 2008) to Social systems(Batty 2007; Chen and Zhan 2008), from Financial systems (Streit and Borenstein 2009) to supply chains (Zarandi et al. 2008), from the modeling of honey bees (Galla 2010) to modeling of traffic lights (Gershenson 2004). In the case of social simulation Agents in agent -based modeling for social simulation may also be given cognition as shown by Sun in (Sun 2006). With such an impressive set of applications, the strength of agent-based modeling (Carmichael 2010) is quite apparent.

One possible explanation of the prevalence of agent -based modeling in such a diverse set of scientific domains is the similarity of models to human Cognition because the ideas inherent to agents is similar to how most humans perceive the surrounding world. In general, agent-based models are particularly useful for developing models of Complex Adaptive Systems. Typical examples of software used to develop agent-based modeling and simulation are NetLogo (Wilensky 1999a, b), StarLogo (Resnick 1996), Repast (North and Macal 2007), MASON (Panait and Luke 2005a, b), Swarm (Pages 2011) and others .

4.1.4 Benefits of Agent-based Thinking

For system modeling involving a large number of interacting entities, at times it is more appropriate to be able to access parameters of each individual "agent". In emerging communication paradigms, network modelers need to model a variety of concepts such as life forms, sensors and robots. Agent-based thinking allows for direct addressability of individual entities or agents. The concept of breeds allows system designer to freely address various system entities. In agent-based modeling and simulation, agents are designed to be addressed for performing a certain action.

Using a type name, agents or "turtles" can be asked to perform actions or change their attributes. Agent-based models are developed with a high level of abstraction in mind. In contrast to programming abstracts such as loops, designers ask agents without worrying about the low-level animation or interaction details necessary for execution. As such, this results in the production of compact programs with a high degree of functionality.

An important benefit of small programs is their ability to greatly reduce the tweak-test-analyze cycle. Thus it is more likely to model complex paradigms within a short time without worrying about the lower layers of other parameters unless they are important for the particular application. As we shall see in this part, it also has great expressive power and most of all, is fun to use. Although being used very frequently to model complex and self-organizing systems it has not previously been used extensively to model computer networks.

4.2 A Review of an Agent-based Tool

In the arena of agent-based tools, a number of popular tools are available. These range from Java based tools such as Mason to Logo based tools such as: StarLogo, NetLogo (Wilensky 1999a, b) etc. Each of these tools has different strengths and weaknesses. In the rest of the part, we focus on just one of these tools: NetLogo as a representative of this set. Building on the experience of previous tools based on the Logo language, NetLogo has been developed from grounds up for complex systems research. Historically, NetLogo has been used for modeling and simulation of complex systems including multi-agent systems, social simulations, biological systems etc., on account of its ability to model problems based on human abstractions rather than purely technical aspects. However, it has not been widely used to model computer networks, to the best of our knowledge.

4.2.1 NetLogo Simulation: An Overview

In this section, we introduce NetLogo and demonstrate its usefulness using a number of modeling and simulation experiments. NetLogo is a popular tool based on the Logo language with a strong user base and an active publicly supported mailing list. It provides visual simulation and is freely available for download and has been used considerably in multi-agent systems literature. It has also been used considerably in social simulation and complex adaptive networks(Vidal et al. 2004). One thing which distinguishes NetLogo from other tools is its very strong user support community. Most times, you can get a reply from someone in the community in less than a day. NetLogo also contains a considerable number of code samples and examples. Most of the time, it is rare to find a problem for which there is no similar sample freely available either within NetLogo's model library or elsewhere from the NetLogo M&S community.

Based on the Logo language, the NetLogo world consists of an interface which is made up of "patches". The inhabitants of this world can range from turtles to links. In addition, one can have user interface elements such as buttons, sliders, monitors, plots and so on.

NetLogo is a visual tool and is extremely suitable for interactive simulations. When one first opens up a NetLogo screen, an interface with a black screen is visible. There are three main tabs and a box called the command center. Briefly, the interface tab is used to work on the user interface manually and the "Information" tab is used to write the documentation for the model. And finally the "procedures" tab is where the code is actually written. The "command center" is a sort of an interactive tool for working directly with the simulation. It can be used for debugging as well as trying out commands similar to the interpreter model which, if successful, can be incorporated in one's program. The commands of a NetLogo procedure can be executed in the following main contexts:

The key inhabitants of the Logo world are the turtles which can be used to easily model network nodes. The concept of agents/turtles is to provide a layer of abstraction. In short, the simulation can address much more complex paradigms which include pervasive models, environment or terrain models or indeed any model the M&S specialist can conceive of without requiring much additional addon modules. However, the tool is extensible and can be directly connected to Java based modules. By writing modules using Java, the tool can potentially be used as the front end of a real-time monitoring or interacting simulation. For example, we could have a java based distributed file synchronization system, which reports results to the NetLogo interface and vice versa, the NetLogo interface could be used by the user to setup the simulation at the backend (e.g. how many machines, how many files to synchronize and subsequently with the help of the simulation, the user could simply monitor the results). Although the same can be done with a lot of other tools and technologies, the difference is that NetLogo offers these facilities almost out of the box and requires minimal coding besides being noncommercial, free and easy-to-install. A single place where the turtle exists is a patch. Observer is a context, which can be used in general without relating to either a patch or a turtle. The NetLogo user manual, which comes pre-packaged with NetLogo, says: "Only the observer can ask all turtles or all patches. This prevents you from inadvertently having all turtles ask all turtles or all patches ask all patches, which is a common mistake to make if you're not careful about which agents will run the code you are writing."

Inside the NetLogo world, we have the concept of agents. Coming from the domain of complex systems, all agents inside the world can be addressed in any conceivable way, which the user can think of, e.g., if we want to change the color of all nodes with communication power <0.5 W, a user can simply say: ask nodes with [power <0.5] [set color green] or if a user wants to check nodes with two link neighbors only, this can be done easily too and so on.

The context of each command is one of three. Observer object is the context, when the context is neither turtle nor the patch. It is called the observer because this can be used in an interactive simulation where the simulation user can interact in this or other context using the command window.

Although there are no real rules to creating a NetLogo program, one could design a program to have a set of procedures which can be called directly from the command center. However, in most cases, it suffices to have user interface buttons to call procedures. For the sake of this part, we shall use the standard technique of buttons.

In this program there will be two key buttons; Setup and the Go buttons. The idea is that the "setup" button is called only once and the "go" button is to be called multiple times (automatically). These can be inserted easily by right clicking anywhere on the interface screen and selecting buttons. So, just to start with NetLogo, the user will need to insert these two buttons in his or her model, remembering to write the names of the buttons in the commands. For the go, we shall make it a forever button. A forever button is a button which calls the code behind itself repeatedly. Now, the buttons show up with a red text. This is actually

```
1. to setup
2. ca ; Clears everything so if we call setup
  again, it won't make a mess
3. crt 100 ; This means we are creating 100
   turtles
4. [
5. setxy random-pxcor random-pycor ;These 100
   turtles, we want them to be spaced out at
  random
6. ; patch x and y co-ordinates
7. ]
8. letmycolor random 140 ; Randomly select a
  color value from 0 to 139
9. ask patches
10.[
11. setpcolormycolor ; Ask all patches to set
   their color to this random color
12.]
13.end
```

Fig. 4.1 Code for setup

NetLogo's way of telling us that the commands here do not yet have any code associated with them. So, let us create two procedures by the name of "setup" and "go". The procedures are written, as shown in Fig. 4.1, in the procedures tab and the comments (which come after a semi-colon on any line in NetLogo) explain the actions that are performed by the commands. This code creates 100 turtles (nodes in this case) on the screen. However the shape is a peculiar triangle by default and colors are assigned at random. Note that we have written code here to have the patches colored randomly.

To create the procedure for the go, the code can be written as listed in Fig. 4.2

Now, if we press setup followed by go, we see turtles walking slowly in a forward direction on the screen, a snapshot of which is shown in Fig. 4.3.

4.2.1.1 Overview of NetLogo for Modeling Complex Interaction Protocols

NetLogo allows for the modeling of various complex protocols. The model, however, does not have to be limited to the simulation of only networks; it can readily be used to model human users, intelligent agents, and mobile robots interacting with the system or virtually any concept that the M&S designer feels worthwhile having in the model. NetLogo, in particular, has the advantage of LISP-like (McCarthy 1965) list-processing features. Thus modeled entities can interact with computer networks. Alternatively, the simulation specialist can interact and create run-time agents to interact with the network to experiment with complex protocols, which are not otherwise straightforward to conceive in terms of programs.

Fig. 4.2 Code for go

```
to go
ask turtles
[
fd 0.001; ask each turtle to move a
small step
]
end
```



Fig. 4.3 Mobile nodes

As an example, let us suppose, if we were to model the number of human network managers (e.g. from 10 to 100) attempting to manage a network of 10,000 nodes by working on workgroups the size of n nodes (e.g. ranging from 5 to 100) at one time while giving a total of 8 h shifts with network attacks coming in as a Poisson distribution; this can be modeled in less than a few hours with only a little experience in NetLogo per se. The simulation can then be used to evaluate policies of shifts to minimize network attacks.

Another example could be the modeling and simulation of link backup policies in case of communication link failures in a complex network of 10,000 nodes along with network management policies based on part-time network managers carrying mobile phones for notification and management versus full-time network managers working in shifts etc. all in one simulation model. And to really make things interesting, we could try these out in reality by connecting the NetLogo model to an actual J2ME based application in Symbian phones using a Java extension; so the J2ME device sends updates using GPRS to a web server which is polled by the NetLogo program to get updates while the simulation is updated in a user interface provided by NetLogo. Again, although the same could be done by a team of developers in a man-year or so of effort using different technologies, NetLogo provides for coding these almost right out of the box and the learning curve is not steep either.

This expressive nature of NetLogo allows modeling non-network concepts such as pervasive computing alongside human mobile users (e.g. in the formation of ad-hoc networks for location of injured humans) or Body Area Networks come in play along with the network. Now, it is important to note here that simulation would have been incomplete without effective modeling of all related concepts which come into play. Depending upon the application, these could vary from ambulances, doctors, nurses to concepts such as laptops, injured humans etc. in addition to readily available connectivity to GIS data provided by NetLogo extensions.

4.2.1.2 Capabilities in Handling a Range of Input Values

Being a general purpose tool, by design, the abstraction level of NetLogo is considered higher. As such, the concepts of nodes, antenna patterns and propagation modeling are all user-dependent. On one hand, this may look burdensome to the user accustomed to using these on a regular basis, as it might appear that he or she will be working a little extra to code these in NetLogo modeling. On the other hand, NetLogo allows for the creation of completely new paradigms of network modeling, wherein the M&S specialist can focus on, for example, purely selforganization aspects or on developing antenna patterns and propagation modeling directly.

4.2.1.3 Range of Statistics and Complex Metrics

NetLogo is a flexible tool in terms of using statistics and measurements. Any variable of interest can be added as a global variable and statistics can be generated based on single or multiple-run. Plots can be automatically generated for these variables as well.

Measurements of complex terms in NetLogo programs are very easy to perform. As an example, if it is required to have complex statistics such as network assembly time, global counters can be used easily for this. Similarly, statistics such as network throughput, network configuration time, throughput delay can be easily modeled by means of similar counters (which need not be integral). By default, NetLogo provides for real-time analysis. Variables or reporters (functions which return values) can be used to measure real-time parameters and the analyst can actually have an interactive session with the modeled system without modifying the code using the "Command Window".

4.3 Verification and Validation of Simulation Models

4.3.1 Overview

Validation of a simulation model is a crucial task (Balci 1998; Banks et al. 2005). Simulations, however well-designed, are always only an approximation of the system and if it was so easy to build the actual system, the simulation approach would never have been used (Law 2008). In traditional modeling and simulation practices, a standard approach to verification and validation (V&V) is the three step approach given by Naylor et al. in (1967) as follows:

- 1. The first step is to develop a model that can intrinsically be tested for a higher level of face validity.
- 2. The next step is to validate the assumptions made in the model
- 3. Finally, the transformations of the input to output from the model need to be compared with those for the actual real-world system.

4.3.2 Verification and Validation of ABMs

While verification and validation are important issues in any simulation model development, in this section, we discuss the peculiarities associated with ABMs in the domain of modeling and simulation of CAS.

Firstly ABMs can be difficult to validate because there is a high tendency of errors and un-wanted artifacts to appear during the development of an ABM as noted by Galan et al. (2009). In addition, since the number of parameters in an ABM model can tend to be quite high, Lucas et al. have noted that it is possible to fall into the trap of tweaking the variables (Lucas et al. 2007).

Bianchi et al. note that validation of agent based models can be quite challenging (Bianchi et al. 2007). Another problem noted by Hodges and Dewar is as to how to ensure that the observed behavior is a true representative of the actual system (Hodges and Dewar 1992). Fagiolo et al. mention four set of issues with Agent-Based models (Fagiolo et al. 2007):

- 1. A "lack of robustness".
- 2. Absence of a high degree of comparability between developed agent-based models.
- 3. A dire shortage of standard techniques for the construction and analysis of agent-based models.
- 4. Difficulties in correlation of the models with empirical data.

Keeping these issues in mind, while validation techniques of agent-based models have been mentioned in some domains such as computational economics and social simulation, there are still a number of open issues:

- 1. There is no standard way of building Agent-based Models.
- 2. There is no standard and formal way of validation of Agent-based Models.
- 3. Agent-Based Modeling and Agent-Based Simulations are considered in the same manner because there is no formal methodology of agent-based modeling (Macal and North 2007).
- 4. Agent-Based Models are primarily pieces of Software however no software process is available for development of such models.
- 5. All validation paradigms for agent-based models are based on quantifying and measurable values but none caters for emergent behavior (Axtell 2000; Axtell et al. 1999) such as traffic jams, structure formation or self-assembly as these complex behaviors cannot be quantified easily in the form of single or a vector of numbers.
- 6. Agent-based models are occasionally confused with multi-agent systems (MAS) even though they are developed for completely different objectives; ABM are primarily built as simulations of CAS, whereas MAS are typically actual software or at time, robotic systems. Although MASs may themselves be simulated in the form of an ABM but that does not change their inherent nature. We would like to note here that differences between MAS and ABMs have been discussed earlier in the part and a further exposition to this effect will be performed in Part III.

4.3.3 Related Work on V&V of ABM

In social sciences literature such as in the case of Agents in Computation Economics (ACE), empirical validation of agent-based models has been described by Fagiolo et al. in (2007). Alternate approaches to empirical validation have been noted by Moss in (2008). Validation of models is closely related to model replication as noted by Wilensky and Rand in (2007). An approach of validation based on philosophical truth theories in simulations has been discussed by Schmid in (2005). Another approach called "companion modeling", an iterative participatory approach where multidisciplinary researchers and stakeholders work together throughout a four-stage cycle has been proposed by Barreteau et al. in (2003).

A different point of view also exists in literature which uses agent-based simulation as a means of validation and calibration of other models such as by Makowsky in (2006). In addition, agent-based simulation has also been shown to be useful in the validation of multi-agent systems by Cossentino et al. in (Cernuzzi et al. 2005).

4.4 Overview of Communication Network Simulators

In this section, an overview of different types of simulators used for the simulation of communication networks is provided.

4.4.1 Simulation of WSNs

Current sensor network simulation toolkits are typically based on simulators such as NS-2, OPNET (Garrido et al. 2008), J-Sim (Sobeih et al. 2005), TOSSIM (Levis et al. 2003) etc. SensorSim is a simulation framework (Park et al. 2000). Amongst traditional network simulations, J-Sim and NS2 have been compared in (Sobeih et al. 2005) and J-Sim has been shown to be more scalable. Atemu (Polley et al. 2004) on the other hand, focuses on simulation of particular sensors. Likewise, TOSSIM (Levis et al. 2003) is a TinyOS Simulator.

4.4.2 Simulation of P2P Networks

In terms of simulation of P2P networks, on one hand, there are actual implementations and on the other, there are simulators of the P2P protocols. These include Oversim (Baumgart et al. 2007) which is based on the OMNET ++ (Varga 2001) simulator. Another simulator for P2P networks is the PeerSim (Jelasity et al. 2008) simulator.

4.4.3 Simulation of Robotic Swarms

In the case of swarm robotics, simulators include Swarm-Bot simulator (Mondada et al. 2004) and WebotsTM robot simulator (Michel 2004). Other simulators include LaRoSim which allows for robotic simulations of large scales (Sahin et al. 2008).

4.4.4 ABM for Complex Communication Networks Simulation

While we have noted above that individual sub-areas of this domain such as WSNs, Swarm robots as well as P2P networks all have dedicated as well as general purpose simulators but all of them are limited to their specific domain, the benefit of using ABM in the modeling and simulation of complex communication networks is that it is a general purpose methodology and thus it can be used to simulate any combination of these in addition to being able to simulate other entities such as humans, plants and animals in the simulation.

4.5 Complex Network Modeling

In this section, an overview of complex network methods is presented. The basic idea of Complex Network Analysis originates from graph theory. A complex network is essentially an advanced graph, where unlike theoretical graphs, each node and edge is loaded with more information. As an example, if we were to develop a social network of friends, the network edges could represent the level of emotions which the friends have for each other. So, if a person Alice considers three people (say Bob, Cassandra and David) as friends, then this could be represented as a network. Suppose Alice considers Cassandra as her best friend so this could be modeled in the network by giving a higher attribute value to the link/edge between Alice and Cassandra. To make things more interesting, the network could be directed so it is possible that Bob might not even consider Alice as a friend. So, each friendship relation should be represented by a directed edge.

Using various Mathematical tools and models, complex networks can be subsequently analyzed and compared with other models from the same or different domains. As an example Barabasi (Albert Laszlo Barabasi 2004) compares Biological networks with models of the world wide web. Besides classification, networks can also be used to discover important features of the numerous nodes (or components) of the CAS. While Complex Networks are a general set of methods, the growth of literature of complex network usage can be identified across various CAS literature ranging from Social Network Analysis (Nooy et al. 2005) to Biological Networks (Junker and Schreiber 2008) and in Citation Networks (Batagelj 2003).

4.5.1 Complex Network Methods

In a CAS, interactions can be modeled as networks. The key difficulty in network design is to understand which data needs to be captured to develop the network model(s). Once the data has been converted to a network, there exist a large number of complex network analysis Mathematical and software tools for performing the analysis. However, the hard part here is the selection of data, the design and extraction of the complex network models. While application of the actual centrality measures appears to be deceptively easy due to the existence of a large set of software tools for assistance, it can be very difficult to actually come up with data which is relevant as well as generates useful networks, which can represent the entire CAS properly. Development of partial networks can result in completely incorrect results as complete networks are required for the accurate calculation of centrality measures (as discussed in the next section). Calculation of centrality measures requires the use of all possible nodes in a connected network.

4.5.2 Theoretical Basis

Graph theory has a long history. One of the earliest known representation of graph problem is the Leonard Euler's "Konigsberg bridge problem" in 1735 which involved representing a map of the river Pregel in the form of a graph (Thulasiraman and Swamy 1992).

A graph G = (V, E) is essentially formed by a set of *vertices* or *nodes* V and a set of *edges* or *arcs* E. Each edge is assigned to two vertices, where the vertices might not be disjunct. Graph nodes as well as edges are given other alpha-numeric attributes including the physical coordinates for display purposes. Networks are typically analyzed using the following methods:

- 1. Global network properties: Since real-world CAS differ from purely randomly generated networks, they can be distinctly categorized using global properties. Three distinct types of network models have been used in literature. The first one is the Erdős-Rényi random network model (Erdős and Rényi 1960). The second model was proposed by Watts and Strogatz by analysis of many real-world networks which they discovered to have a smaller average shortest path length coupled with a high clustering coefficient as compared with random networks. These networks are labeled the Watts and Strogatz small-world model (Watts and Strogatz 1998) after their discoverers. Another model, called the scale-free network model was proposed by Barabási and Albert (1999) based on ideas of complex networks from real-world CAS domains. These networks exhibit some degree of a power law distribution in the "degree centrality". This implies that they contain very few nodes with a higher degree and a large number of nodes with a lower degree.
- 2. Network centralities: Unlike global network properties, centralities deal with particular nodes. As such, using a centrality analysis, different nodes can be ranked according to their importance in *Centrality indices*. It is pertinent to note that not all centrality measures might give substantial results for a particular network. As such, it is typical to develop numerous networks as well as perform considerable analysis by trial and error before a particular extraction of network as well as a centrality measure is discovered showing significant results.
- 3. Network motifs: Motifs are commonly used network architectural patterns. They are often used in CAS modeling to discover particular patterns of local interactions. Examples include signal transduction (Hulett 1996) and gene regulatory biological networks (Davidson 2006). Recent work includes (Davidson 2010) who has demonstrated emerging properties in Gene regulatory networks.
- Network clustering: Biological networks have been studied in the form of hierarchical structures with motifs and pathways at lower levels to functional molecules for large scale organization of networks by Oltvai and Barábasi (2002).

4.5.3 Centralities and Other Quantitative Measures

In this section, a description of some of the commonly used quantitative measures in complex networks is provided.

4.5.3.1 Clustering Coefficient

The clustering coefficient is a means of quantitative measurement of the local cohesiveness in a complex network. It is a measure of the probability that two vertices with a common neighbor are connected.

The formula for calculation of the clustering coefficient is given as follows:

$$Ci = \frac{2Ei}{ki(ki-1)} \tag{4.1}$$

where

 E_i = number of edges between neighbors of a node i

 k_i = degree of the node i

The global/mean clustering coefficient $C = \langle C_i \rangle$ is found by taking an average of all the clustering coefficients.

4.5.3.2 Matching Index

Matching index gives a quantitative means of measuring the number of common neighbors between any two vertices. In other words, for empirical networks, two functionally similar vertices need not be directly connected with each other. It is formally defined as following:

$$M_{ij} = \frac{N_{k,l}A_{ik}A_{jl}}{k_i + k_j - N_{k,l}A_{ik}A_{jl}}$$
(4.2)

Where the numerator represents the common neighbors while the denominator represents the total number of neighbors of the two nodes i and j.

4.5.4 Centrality Measures

A centrality is formally defined as a function $C: V \mapsto R$ for a directed or undirected graph G = (V, E)(Junker and Schreiber 2008). A centrality is a real number assigned to each vertex allowing for a pair-wise comparison across the entire network.

4.5.4.1 Degree Centrality

Degree centrality or simply "degree" of a node is a basic centrality measure which identifies the connections of a node with other nodes. For directed networks, there can be two kinds of degree centrality measures. The in-degrees and the out-degrees can be found by the summation of the total in-links and the total out-links respectively. Degree centrality is regarded as a local centrality measure however nodes having a higher degree can be more important as compared with nodes with a lower degree. As such, deletion of high degree nodes can disrupt the network structure and flow of interactions.

4.5.4.2 Eccentricity Centrality

Eccentricity of a node v is defined as the maximum distance between v and u for all nodes u. Eccentricity centrality assists in computation of the maximum distance, which can be defined as the length/distance of the longest shortest path to all other vertices present in the network. Nodes which are easily reachable from other nodes receive the highest value. Eccentricity identifies the node that can be reached within equal distance from all other nodes in the network. Mathematically, eccentricity can be defined as:

$$Cecc(s) = \frac{1}{\operatorname{Max}\{dist(s,t)\}}$$
(4.3)

where

s and t are the nodes belonging to the set of vertices V

4.5.4.3 Closeness Centrality

Closeness centrality is similar to eccentricity but utilizes the minimum distance from a target node to all other nodes within the network.

The formula for the calculation of the closeness centrality is of a node *s* for all nodes *t* is given as follows:

$$Cclo(s) = \Sigma \frac{1}{dist(s,t)}$$
(4.4)

4.5.4.4 Shortest Path Betweenness Centrality

It is calculated by measuring the number of times a particular node comes in the shortest path between any two nodes. In other words, it identifies the ability of a node to monitor communication across the network. A higher value implies a better ability of a particular node to monitor network communication. Mathematically it can be defined as:

$$Cspb(v) = \Sigma \frac{\sigma st(v)}{\sigma st}$$
(4.5)

where

 $\sigma st(v)$ is the number of the shortest paths between nodes s and t containing the vertex v between the nodes

 σ stis the total number of the shortest paths present between two nodes s and t

4.5.5 Software Tools for Complex Networks

While Complex Network Analysis uses a number of mathematical tools, some of which have been described in this part, for practical reasons, network scientists use a number of software tools for performing network operations. These include network construction, extraction, simulation, visualization and analysis tools such as Network Workbench (Team 2006), Pajek (Batagelj and Mrvar 1998) and Citespace (Chen 2006), Cytoscape (Shannon et al. 2003), Visone (Baur et al. 2002) and others.

4.6 Conclusions

In this part, we have discussed the background and related work required for an understanding of the subsequent chapters. We have discussed modeling and simulation and its relation to CAS research. In the next part, we present complex network modeling level of the proposed framework, which is concerned with developing Complex Network models and performing Complex Network Analysis of large amounts of CAS interaction data.

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