Department of Mathematics and Systems Analysis

Bayesian Networks, Influence Diagrams, and Games in Simulation Metamodeling

Jirka Poropudas

Aalto University

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Jirka Poropudas

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Abstract

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Abstract
The Dissertation explores novel perspectives related to time and conflict in the context of simulation metamodeling referring to auxiliary models utilized in simulation studies. The techniques innovated in the Dissertation offer new analysis capabilities that are beyond the scope of the existing metamodeling approaches. In the time perspective, dynamic Bayesian networks (DBNs) allow the probabilistic representation of the time evolution of discrete event simulation by describing the probability distribution of the simulation state as a function of time. They enable effective what-if analysis where the state of the simulation at a given time instant is fixed and the conditional probability distributions related to other time instants are updated revealing the conditional time evolution. The utilization of influence diagrams (IDs) as simulation metamodels extends the use of the DBNs into simulation based decision making and optimization. They are used in the comparison of decision alternatives by studying their consequences represented by the conditional time evolution of the simulation. For additional analyses, random variables representing simulation inputs can be included in both the DBNs and the IDs. In the conflict perspective, the Dissertation introduces the game theoretic approach to simulation metamodeling. In this approach, existing metamodeling techniques are applied to the simulation analysis of game settings representing conflict situations where multiple decision makers pursue their own objectives. Game theoretic metamodels are constructed based on simulation data and used to study the interaction between the optimal decisions of the decision makers determining their best responses to each others' decisions and the equilibrium solutions of the game. Therefore, the game theoretic approach extends simulation based decision making and optimization into multilateral settings. In addition to the capabilities related to time and conflict, the techniques introduced in the Dissertation are applicable for most of the other goals of simulation metamodeling, such as validation of simulation models. The utilization of the new techniques is illustrated with examples considering simulation of air combat. However, they can also be applied to simulation studies conducted with any stochastic or discrete event simulation model.

Keywords Simulation, simulation metamodeling, discrete event simulation, stochastic simulation, Bayesian networks, influence diagrams, game theory

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Tiivistelmä

Väitöskirjassa tarkastellaan kahden uuden aikaan ja konflikteihin liittyvän näkökulman yhdistämistä simulaatiometamallinnukseen, jossa tilastollisia apumalleja hyödynnetään osana simulaatiotutkimusta. Väitöskirjassa esiteltävät tekniikat tarjoavat uusia analyysitapoja, jotka eivät ole mahdollisia olemassa olevilla mallinnustekniikoilla. Aikanäkökulmaan liittyen dynaamiset Bayesverkot (DBN) mahdollistavat diskreetin tapahtumasimuloinnin etenemisen kuvailemisen esittämällä simulaation tilan todennäköisyysjakauman ajan funktiona. Niiden avulla voidaan toteuttaa tehokkaasti "mitä jos"-analyyseja, joissa simulaation tila kiinnitetään annetulla ajanhetkellä ja simulaation ehdollista kehitystä tarkastellaan päivittämällä toisia ajanhetkiä kuvaavat ehdolliset todennäköisyysjakaumat. Vaikutuskaavioiden (ID) hyödyntäminen simulaatiometamalleina laajentaa DBN:ien käytön simulaatioperusteiseen päätöksentekoon ja optimointiin. Vaikutuskaavioilla voidaan vertailla päätösvaihtoehtoja ja tutkia niiden seuraamuksia kuvaavia ehdollisia simulaation kulkuja. Sekä DBN:iin että ID:hin voidaan sisällyttää simulaatiosyötteitä kuvaavia satunnaismuuttujia. Konfliktinäkökulmaan liittyen väitöskirja laajentaa simulaatioperusteisen päätöksenteon ja optimoinnin monen toimijan asetelmiin esittelemällä peliteoreettisen lähestymistavan simulaatiometamallinnukseen. Tässä lähestymistavassa olemassa olevia metamallinnustekniikoita sovelletaan konfliktitilanteita kuvaavien peliasetelmien simulaatioanalyyseihin, joissa useat toimijat tavoittelevat omia tavoitteitaan. Peliteoreettisten metamallien avulla tutkitaan toimijoiden pelioptimaalisten päätösten välisiä riippuvuuksia ja niistä seuraavia pelin tasapainoratkaisuja. Aikaan ja konflikteihin liittyvien sovellusmahdollisuuksien lisäksi väitöskirjassa esiteltävät tekniikat ovat sovellettavissa myös useimpiin muihin simulaatiometamallien käyttötarkoituksiin, kuten simulaatiomallien validointiin. Uusien tekniikoiden hyödyntämistä on esitelty ilmataistelua kuvaavien simulaatioesimerkkien avulla. Tekniikat soveltuvat myös muita ilmiöitä kuvaavien stokastisten simulaatioiden ja diskreettien tapahtumasimulaatioiden analysointiin.

Avainsanat Simulointi, simulaatiometamallinnus, diskreetti tapahtumasimulointi, stokastinen simulointi, Bayes-verkot, vaikutuskaaviot, peliteoria

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Publications

The Dissertation consists of the present summary article and the following papers:

[I] J. Poropudas and K. Virtanen. Simulation Metamodeling with Dynamic Bayesian Networks. *European Journal on Operational Research*, 214:(3)644–655, Nov. 2011.

[II] J. Poropudas and K. Virtanen. Simulation Metamodeling in Continuous Time using Dynamic Bayesian Networks. *Proceedings of the 2010 Winter Simulation Conference*, pages 935–946, Baltimore, MD, 2010.

[III] J. Poropudas and K. Virtanen. Analyzing Air Combat Simulation Results using Dynamic Bayesian Networks. *Proceedings of the 2007 Winter Simulation Conference*, pages 1370–1377, Washington, DC, 2007.

[IV] J. Poropudas and K. Virtanen. Influence Diagrams in Analysis of Discrete Event Simulation Data. *Proceedings of the 2009 Winter Simulation Conference*, pages 696–708, Austin, TX, 2009.

[V] J. Poropudas and K. Virtanen. Game Theoretic Validation and Analysis of Air Combat Simulation Models. *IEEE Transactions on Systems, Man, and Cybernetics – Part A: Systems and Humans*, 40(5):1057–1070, Sep. 2010.

[VI] J. Pousi, J. Poropudas, and K. Virtanen. Game Theoretic Simulation Metamodeling using Stochastic Kriging. *Proceedings of the 2010 Winter Simulation Conference*, pages 1456–1467, Baltimore, MD, 2010.

Contributions of the author

The author was the main contributor in developing the simulation metamodeling techniques based on dynamic Bayesian networks and influence diagrams in Papers [I]-[IV]. The development of the game theoretic metamodeling approach presented in Paper [V] was carried out in collaboration with Dr. Kai Virtanen. The application of stochastic Kriging to game theoretic simulation metamodeling in Paper [VI] was suggested by the author. The implementation of the metamodels as well as the computation and analysis of the results were performed by the author in Papers [I]-[V]. In Paper [VI], the analyses were carried out by Mr. Jouni Pousi. The author was the principal writer in Papers [I]-[V] and had an active role in the writing of Paper [VI].

Preface

This Dissertation has been made possible by several people, whom I have the privilege to acknowledge here.

First and most importantly, I want to thank my supervisor Adjunct Professor Kai Virtanen for the his support and contributions during the work. I believe that his emphasis on the clarity of writing has greatly improved not only this Dissertation but also my way of thinking. Now I know that you appear like fool, if you can not express yourself in an understandable manner. I have also learned that sometimes the best and the only way to get your point across is to yell louder than the opposite side. Second, I have to thank my supervising professor Raimo P . Hämäläinen, for his contributions and the possibility of working at the Systems Analysis Laboratory. Third, I thank my co-author Mr. Jouni Pousi who is the hardest working man in show business. I also appreciate greatly the preliminary examiners of the Dissertation, Dr. Ken R. McNaught and Dr. Joel Brynielsson, and their insightful comments and ideas for improvement.

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Helsinki, October 2011

Jirka Poropudas

Contents

1 Introduction

The Dissertation approaches simulation metamodeling, referring to input-output models auxiliary to simulation models (e.g., Friedman 1996; Barton 1998; Kleijnen 2008), from two novel perspectives: time and conflict. The time perspective is examined with techniques provided by the methodology of Bayesian networks (Pearl 1986; Dean and Kanazawa 1990; Jensen and Nielsen 2007) and influence diagrams (Howard and Matheson 1984, 2005) while the conflict perspective is studied using game theory (von Neumann and Morgenstern 1944; Fudenberg and Tirole 1991; Başar and Olsder 1995). Simulation is a versatile and widespread analysis methodology where simulation models are applied to the study of systems whose analysis would otherwise be overtly difficult, expensive, or dangerous, such as air combat (see, e.g., Law 2006). The utilization of simulation metamodels for representing the dependence between simulation inputs and outputs is motivated by the complexity of the related simulation models and the inconvenience of the direct analysis of simulation data. The new techniques based on Bayesian networks, influence diagrams, and game theory enable the analysis of the internal dynamics of simulation models as well as the consideration of simulation models related decision making problems with multiple decision makers. Such analyses are beyond the capabilities of the existing simulation metamodels.

In simulation, the operation of a real-world or conceptual system is imitated by generating a sample of artificial histories of the system (Banks 1998b). It is used to analyze the behavior of systems, study what-if questions, and aid in system design (Law 2006). Simulation models are controlled using simulation input variables whose values are collected into a simulation data set together with observed simulation outputs. The data are then used to draw inferences concerning the operating characteristics of systems (Banks 1998b). Nowadays, simulation is one of the most widely used techniques in operations research and management science (Law 2006) where the studies of all but the most elementary systems rely on sampling experiments performed on computers (Fishman 1996). Other application areas of simulation include, among others, chemistry, engineering, physics, and statistics. More detailed introductions to simulation are given by, e.g., (Banks 1998a; Law 2006).

The Dissertation focuses on stochastic simulation where systems with internal uncertainties and random factors are studied. In particular, a branch of stochastic simulation called discrete event simulation (DES, see, e.g., Law 2006; Banks et al. 2009) is discussed. Such simulation models are analyzed using the Monte Carlo method (e.g., Fishman 1996) where the effects of random factors are studied by generating artificial samples of random variables using pseudo-random numbers. The metamodeling techniques introduced in the Dissertation allow new possibilities for analysis of such simulation models. The utilization of these techniques is illustrated with examples dealing with air combat simulation.

Even though modern simulation analyses invariably involve computers, the use of simulation as an analysis tool precedes computers. The earliest documented study utilizing "artificial sampling" is the classical study performed by count Buffon in 1777 in which a manual Monte Carlo method is employed to estimate the value of π (de Buffon 1777). During the World

War II, the newly developed digital computers offered the computational capabilities needed in performing simulation studies which, together with the introduction of the Monte Carlo method, led to the rapid growth of the field of simulation. The Monte Carlo method was introduced by S. Ulam, J. von Neumann, N. Metropolis, and others who suggested that sampling experiments executed on digital computers provide solutions to analytically intractable problems (Fishman 1996). The seminal articles on stochastic simulation (Conway et al. 1959; Conway 1963) separate simulation analysis into two parts, viz., model construction and model analysis, which holds even today. In the following decades, simulation methodology experienced tremendous growth both in importance and in area of application. A more extensive presentation of the history of simulation is found, e.g., in (Goldsman et al. 2010).

The increasing popularity of simulation and the complexity of problems under consideration has also called for advances in the methodology applied to the analysis of simulation data. For this purpose, simulation metamodels (see, e.g., Friedman 1996; Barton 1998; Kleijnen 2008), i.e., statistical auxiliary models, have been introduced to describe the dependence between simulation inputs and outputs. The metamodels are used for the simplification and interpretation of the simulation model in order to increase understanding about the system under consideration. More practical uses of the simulation metamodels include sensitivity and what-if analyses as well as prediction and optimization of simulation outputs.

The initial articles on simulation metamodeling (Mihram 1970; Racite and Lawlor 1972; Biles 1974) deal with the values of simulation input that yield the optimal simulation output. Experimental design and sensitivity analysis as well as the term "metamodel" are first discussed in the simulation context in (Blanning 1974, 1975a,b). Linear regression models as simulation metamodels are introduced and studied in (Kleijnen 1975, 1979; Kleijnen et al. 1979; Kleijnen 1987) as well as in (Hopmans and Kleijnen 1980). More recent additions to simulation metamodeling methodology include, among others, neural networks (Fishwick 1989), spline models (Friedman 1991), and stochastic Kriging (Ankenman et al. 2010). For a more detailed review of simulation metamodeling, see, e.g., (Barton 1998).

The new analysis capabilities offered by the techniques introduced in the Dissertation involve the time evolution of discrete event simulation and simulation models representing conflict situations with multiple decision makers. The time evolution is studied using Bayesian networks (BNs, Pearl 1986; Jensen and Nielsen 2007) and, in particular, dynamic Bayesian networks (DBNs, Dean and Kanazawa 1990). The DBN metamodels offer a graphical, functional, and numerical presentation for the joint probability distribution of random variables representing the simulation state at different time instants. The DBNs enable various analyses which are time-consuming if conducted directly based on simulation data. In simulation based decision making and optimization, influence diagrams (IDs, Howard and Matheson 1984, 2005), which are a decision theoretical extension of BNs, are used as simulation metamodels.

In the Dissertation, simulation metamodels based on game theory (von Neumann and Morgenstern 1944) are introduced as tools for analysis of conflict situations where multiple decision makers, viz., players, pursue their individual objectives whose attainment is measured with payoff functions. The game setting and the interaction between the players follow from the fact that the players try to maximize their own payoffs that depend also on the decisions made by other players. The game theoretic approach is now applied to existing metamodeling techniques, such as regression models and stochastic Kriging, which enables their utilization in analysis of multilateral decision settings. For a more detailed presentation of game theory, see, e.g., (Fudenberg and Tirole 1991; Başar and Olsder 1995).

The construction and utilization of the metamodeling techniques presented in the Dissertation are illustrated using examples related to discrete event simulation of air combat. All the techniques are also applicable to other kinds of simulation models which is demonstrated by presenting simpler academic examples such as the simulation of Poisson processes and queues. The new techniques also serve as basis for further advances, such as the utilization of multi-criteria influence diagrams (e.g., Diehl and Haimes 2004) as simulation metamodels.

This summary article is structured as follows. Section 2 gives a short introduction to simulation methodology including discussion on representing systems with simulation models and their analysis. In Section 3, simulation metamodeling is discussed and the most widely used simulation metamodeling techniques are introduced. The contribution of the Dissertation is summarized in Section 4. In Section 5, conclusions are given and directions for future research are pointed out.

2 Simulation

As stated in Section 1, simulation refers to a methodology where computers are used to imitate the operations of real-world or conceptual facilities or processes which are now referred to as systems. In practice, what is referred to as "the system" depends on the context of the particular study. For example, in air combat simulations discussed in the Dissertation, the system consists of pilots, aircraft, weapons systems, radars, and other hardware. In a more general setting, a system is defined as a collection of entities or components, e.g., people or machines, that act and interact together towards the accomplishment of some logical end (Law 2006). A system is often influenced by its environment through various inputs describing, e.g., alternative system settings or configurations as well as different operational environments (Banks et al. 2009). These inputs can be either controls applied to the system or uncontrollable environmental factors. The behavior of the system can be described as an input-output mapping where the system is affected by inputs which results in a certain response, i.e., the system output (Friedman 1996).

Figure 1 presents alternative ways to study a system in order to, e.g., gain insight to the relationships between its components or to predict its behavior under given settings (Law 2006). If it is possible to alter the system physically and then let it operate under the new settings, the system itself may be used for experimentation and collecting data. However, in practice, such an experiment may be too costly, disruptive, or even dangerous. On the other hand, the system may exist only on conceptual level and the objective of the study could be to select the best configuration to be used in the construction of the physical system. For these

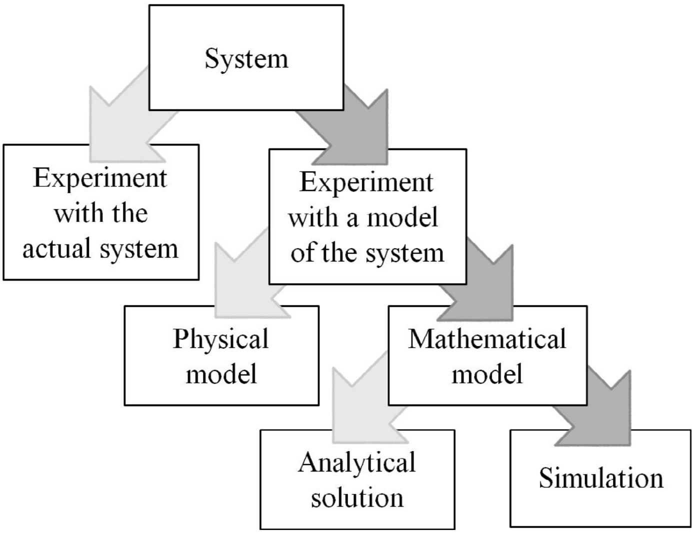

Figure 1: Ways to study a system (Law 2006).

reasons, it may be necessary to build a model for the system, i.e., an artificial construction that imitates the input-output mapping of the system and enables the required analysis.

The model can be a physical model, e.g., used in studying the aerodynamic properties of an aircraft in wind tunnel experiments, or a mathematical model. Mathematical models represent the system in terms of logical and quantitative relationships (Law 2006). If the mathematical model is simple enough, it can be studied with mathematical methods to obtain an exact solution, i.e., an analytical solution, to the problem at hand. This way of studying the model and the corresponding system is desirable, if such a solution is available (Law 2006).

However, most real-world systems are large, dynamic, complex, and involve various uncertainties. Therefore, their modeling is usually more difficult than modeling a strictly physical system (Pritsker 1998) and the resulting models are too complex to be evaluated analytically. These kind of systems are studied numerically by means of simulation. In practice, the model is converted into a computer program. The utilization of simulation in solving problems provides flexibility to build either aggregate or detailed models (Pritsker 1998). In the following, brief introductions to the key concepts of simulation modeling including the categorization of simulation models as well as the practical execution of a simulation study are given.

2.1 Simulation Modeling

Simulation models can be either static or dynamic. In a dynamic simulation model, the time evolution of a system is taken into account as the state of the model changes in time (Law

2006). Such models can be further classified based on the time advancement mechanism employed. In discrete time models, the simulation state is updated at fixed time increments. Continuous time models represent systems whose state changes continuously in time, e.g., following a set of differential equations (Law 2006). On the other hand, simulation models can be categorized into deterministic and stochastic. The former models represent systems without inherent uncertainty. In such simulations, a fixed set of inputs will result in a fixed set of outputs. Stochastic simulation models, on the other hand, include random factors and uncertainties. Therefore, their outputs are random observations of the characteristics of the system in question. In simulation studies, simulation models can also be classified as inexpensive or expensive depending on their required running times. However, such a division depends also on the purposes of the study and available computer resources.

In the context of military training including, e.g., air combat, simulation models are categorized into live, virtual, and constructive simulation models (Hill et al. 2001). In this classification, live simulation refers to real people using real systems, e.g., in flight exercises between friendly pilots. In virtual simulations, real people control simulated systems, e.g., pilots practicing with "man in the loop" air combat simulators. In constructive simulation, also the human elements of the system are included in the simulation model. That is, the performance of simulation runs does not necessitate human involvement. The air combat analyses presented in the Dissertation involve a discrete event simulation model that falls into the latter category.

Discrete event simulation (DES, see, e.g., Law 2006; Banks et al. 2009) is the most widely used approach to the simulation of dynamic and stochastic systems. In DES, the time evolution of a system is treated in continuous time but the values of simulation state variables change instantaneously at discrete time instants. These changes are called events. Typically, DES models do not include an outside operator, i.e., they are constructive in nature. A classical example of DES is a queuing model (Law 2006), where the state of simulation is determined by the number of customers in the queue and the statuses of servers, while the simulation events comprise of the arrivals and the departures of the customers. The example analyses conducted in the Dissertation are based on an air combat simulation model called X-Brawler (L-3 Communications Analytics 2002) that employs DES.

As mentioned in Section 1, stochastic simulation models are studied using the Monte Carlo method (Law 2006; Fishman 1996) which is a simulation scheme where the effects of random factors and uncertainties are studied by generating artificial samples of random variables using pseudo-random numbers (Kleijnen 2008). The method can be used to solve problems with inherent probabilistic structure and those with no probabilistic basis. Thus, in addition to simulation, it is applied for obtaining approximate solutions to a variety of mathematical problems. In the Dissertation, the Monte Carlo method is employed in the context of DES when analyzing air combat using X-Brawler. One should note that some authors, e.g., (Law 2006), limit the term "Monte Carlo simulation" to static simulation models.

The Monte Carlo method relies on computer algorithms for generating pseudo-random samples from suitable probability distributions. The most convenient and reliable way of generating random numbers for stochastic simulations is the utilization of deterministic algorithms with a solid mathematical basis. These algorithms do not, in fact, produce random numbers, but pseudo-random numbers, i.e., sequences of numbers which seem to behave like independent random numbers (L'Ecuyer 1998). A review of desirable properties of pseudo-random number generators as well as of existing algorithms is found in (L'Ecuyer 1998). The generation of random samples of variables with given probability distributions is discussed in (Cheng 1998). By producing a large enough artificial sample of observations, the Monte Carlo method provides a specified accuracy of results. Furthermore, the running times of Monte Carlo simulations can be condensed with numerous techniques discussed in, e.g., (Law 2006; Fishman 1996).

In practice, a simulation model is implemented into a computer code that produces the simulation outputs for given values of inputs. The development of simulation models can be carried out using general purpose programming languages, such as FORTRAN, C, C++, and Java. Additionally, there exist numerous programming languages designed especially for simulation, examples being GPSS/H and SIMAN V. Furthermore, there are various simulation software, e.g., AnyLogic, Arena, and SIMUL8, that offer graphical user interfaces, animation, and automatic collection of simulation outputs. These software also include tools for analyzing simulation outputs either graphically or statistically. Note that all the listed programming languages and simulation software have their individual strengths and areas of application. Finally, there are a myriad of commercial simulation models tailored for particular applications, such as X-Brawler used in the Dissertation. In the Dissertation, all the simulation models not related to air combat are implemented using MATLAB (Mathworks 2011). For a comprehensive discussion of simulation languages and software, see, e.g., (Banks et al. 2009). Reviews of history of simulation languages and software are given by, e.g., (Nance and Sargent 2002; Robinson 2005; Goldsman et al. 2010).

2.2 Simulation Analysis

In the context of stochastic simulation, a simulation study can be decomposed into the four steps illustrated in Figure 2 by adapting the outline presented in (Friedman 1996). An example of a complete simulation study is presented, e.g., in (Mattila et al. 2008). In the *simulation model construction*, the scope of the system and the objectives for the simulation study are defined. In the design of the simulation model, the system under consideration is first presented as a conceptual model including a series of mathematical and logical relationships concerning the components and the structure of the system. The conceptual model also determines the inputs and outputs of the simulation model. The simulation model is implemented by writing a computer code based on the conceptual model using a suitable programming language or simulation software. The resulting simulation model is verified, i.e., it is confirmed that the computer code implements the conceptual model correctly, as well as validated, i.e., it is ascertained that the simulation model represents the system at an acceptable accuracy (Balci 1998; Sargent 2010).

1. Simulation model construction
   a) Problem definition
   b) System analysis and data collection
   c) Design of simulation model
   d) Building simulation model including verification and validation
2. Simulation experiment
   a) Experimental design
   b) Running simulations
3. Analysis of simulation data
   a) Statistical analysis of simulation data
   b) Building metamodel
4. Utilization of simulation results
   a) Decision making and optimization
   b) Implementation

Figure 2: Steps of a simulation study using stochastic simulation (adapted from Friedman 1996).

After the simulation model has been constructed, a *simulation experiment* is conducted. A suitable experimental design is defined by determining the combinations of the values of simulation inputs, i.e., the design sites, to be studied. The purpose of the experimental design is to extract as much relevant information as possible from the simulation runs (Kleijnen 1998; Barton 2008; Kleijnen 2008). It also determines, e.g., the number of simulation runs and run lengths for individual simulations. Then, the simulation runs are performed according to the experimental design. The values of simulation inputs and the corresponding values of simulation outputs are collected into a simulation data set.

Next, the *analysis of simulation data* is conducted. The outputs of a stochastic simulation model are realizations of random variables and, therefore, suitable statistical techniques are employed (Alexopoulos and Seila 1998; Alexopoulos 2006, 2007). For example, multivariate techniques are used (Friedman 1987; Charnes 1991, 1995), if the study involves multiple simulation outputs. On the other hand, one can also utilize simulation metamodels – the topic of the Dissertation – for analyzing the simulation data. The construction and utilization of such metamodels are discussed in more detail in Section 3.

The statistical analysis of simulation data as well as simulation metamodels provide *simulation results* that are utilized in various ways in simulation based decision making where simulation is used to examine the characteristics of a system. On the most fundamental level, the simulation studies increase the understanding about the system under consideration and provide additional insight to decision problems related to the system. For example, alternative system configurations can be compared using what-if analysis to find the best alternative.

In simulation optimization (Azadivar 1999; Ólafsson and Kim 2002; Cheng and Holland 2004; Fu et al. 2005), the aim is to determine the system settings that produce desired results, i.e., the values of simulation inputs that lead to the optimal values of simulation outputs. A number of approaches have been proposed for simulation optimization, such as ranking and selection (Goldsman 1998; Swisher and Jacobson 1999; Kim and Nelson 2005), metamodel based methods (Kleijnen 1998; Barton and Meckesheimer 2006), gradient based procedures (Fu 2005), and others (see, e.g., Rubinstein and Shapiro 1993; Andradóttir 2005; Ólafsson 2005). Reviews of methods used for combining simulation and optimization are given in (April et al. 2003; Fu et al. 2005). Overall, the simulation based decision making can be based on raw simulation data or a suitable simulation metamodel, such as the new metamodels presented in the Dissertation, can be utilized. In the following, a brief introduction to simulation metamodeling is given.

3 Simulation Metamodeling

A simulation model, although simpler than a real-world system, can still be a complex way of relating system input to output. To avoid this inconvenience, simulation metamodels (see, e.g., Friedman 1996; Barton 1998; Kleijnen 2008) are used to aid simulation analyses. Simulation metamodels are also referred to as response surfaces (Montgomery 1977), surrogate models (Yeşilyurt and Patera 1995), emulators (Conti and O'Hagan 2010), auxiliary models (Michaelides and Ng 2000), or repro-models (Meisel and Collins 1973).

The objective of simulation metamodeling is to reproduce the input-output mapping described by the simulation model as well as to provide a framework for studying the behavior of the system under consideration. If the running times of simulations are a limiting factor, metamodels can be used as a time saving measure to predict simulation outputs for simulation inputs. On the other hand, in studies where simulation data are abundant, metamodels concentrate and refine the input-output data into a more manageable form while retaining the significant features and properties of the simulation model. Finally, simulation metamodels are easy to use and their analysis does not require special know-how which may be the case for some simulation models. The simulation metamodeling adds another level of abstraction to the simulation study as it is a statistical representation or some other approximation for input-output function defined by the underlying simulation model. The levels of abstraction related to a simulation study are illustrated in Figure 3.

Simulation inputs used in simulation describe the inputs of a system, i.e., the factors affecting the system under consideration. In practice, the simulation inputs are variables and parameters defining the configuration of the simulated system. All inputs of the system are not necessarily included in the simulation model. The simulation metamodel is constructed for one or more inputs of interest at a time. That is, its inputs do not necessarily involve all inputs of the simulation model. Similar relationship holds also for the outputs: the simulation model usually produces observations on only some of the outputs of the system and only a subset of these outputs is included in the metamodel. For several simulation outputs, multiple

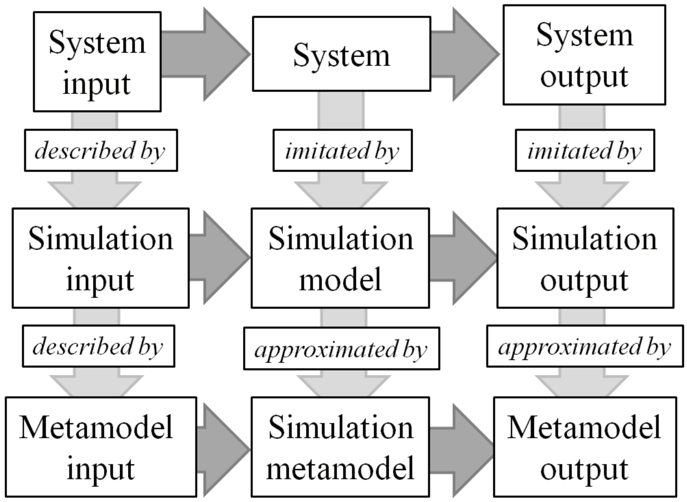

Figure 3: Levels of abstraction in a simulation study and the related input-output mappings.

metamodels can be constructed in parallel.

The characteristics of simulation inputs are determined by the simulation model and their values by the experimental design while the definition of a simulation output is more relaxed. Typically, simulation outputs are used to estimate expected values by calculating time averages of simulation state variables, e.g., the average length of a queue, or the average values of simulation state variables at the end of the simulation, e.g., the outcome of an air combat. In such cases, the outputs of a metamodel give estimates for the expected values of the corresponding simulation outputs. Nevertheless, in a more general setting, the simulation output may include any outputs produced by the simulation model regarding its state. For example, in the DBN metamodels discussed in the Dissertation, the simulation outputs are associated with time series representing the simulation state during the simulation.

In the following, an introduction to the goals of simulation metamodeling as well as the construction of metamodels is given. Then, a variety of simulation metamodel types are briefly reviewed.

3.1 Goals of Simulation Metamodeling

Simulation metamodels can be utilized for multiple purposes in order to increase understanding about the system under consideration. In the earliest articles on simulation metamodeling, simulation metamodels are used to obtain sensitivity information (Blanning 1974). Here, sensitivity information refers to comparison of decision alternatives, identification of quantifiable and unquantifiable advantages of alternatives, experimentation with environmental variables, also known as what-if analysis, and exploring the effects of controllable variables. These exercises are still relevant which is seen in Table 1 where the main goals for the utilization of simulation metamodels are summarized and classified according to their analytical perspectives.

Table 1: Goals of simulation metamodeling.

System perspective	Simulation metamodels ...
Understanding the behavior of the system	Offer a compact representation for the underlying system revealing its dynamics and behavior
Hypotheses testing	Aid in testing hypotheses about the system
Generalization to other systems	May be applicable in analysis of other similar systems
Simulation perspective	**Simulation metamodels ...**
Simplification of the simulation model	Are easier and less time-consuming to apply than the simulation model
Interpretation of the simulation model	Describe transparently the behavior and dynamics of the simulation model
Verification and validation of the simulation model	Make simulation data easier to interpret which is useful in verification and validation of the simulation model
Input-output perspective	**Simulation metamodels ...**
Prediction of outputs	Predict values of outputs without additional simulations
Sensitivity analysis	Describe the effect of changes in inputs on outputs
What-if analysis	Express the effects of alternative values of inputs on outputs
Inverse questions	Solve the values of inputs that produce the given values of outputs
Optimization of outputs with respect to inputs	Find the values of inputs that produce the optimal values of outputs

From the *system perspective*, simulation metamodels describe the behavior and dynamics of the system. In this perspective, certain hypotheses about the nature of the system can be tested and the conclusions may also be generalized to similar systems. In the *simulation perspective*, metamodels simplify the utilization of the simulation model which aids its interpretation, verification, and validation. Finally, input-output mappings provided by metamodels are used in various analyses regarding the interdependence between the inputs and the outputs. From this *input-output perspective*, the most important exercises are the prediction of outputs, sensitivity analysis, and optimization of outputs. For further discussion of the motivation for simulation metamodeling, see also (Friedman 1996; Kleijnen and Sargent 2000; Kleijnen 2008).

3.2 Construction of Simulation Metamodels

Regardless of the goal of a simulation study or the type of simulation metamodel to be implemented, the construction of a simulation metamodel follows the sequence of steps presented in Figure 4 (Kleijnen and Sargent 2000). This sequence is also proper for the metamodeling techniques presented in the Dissertation.

1. Problem structuring
   a) Determine goals
   b) Identify inputs
   c) Determine experimental region
   d) Identify outputs
   e) Specify desired accuracy
2. Metamodel specification
3. Simulation experiment
   a) Experimental design
   b) Data collection
4. Metamodel construction
5. Metamodel validation

Figure 4: Construction of a simulation metamodel (adapted from Kleijnen and Sargent 2000).

The goal of the metamodeling is determined in the *problem structuring* (see, Table 1). Here, the discrete or continuous simulation inputs that are to be included in the metamodel are also identified. The experimental region, i.e., the range of possible values for the simulation inputs, determines the domain of the metamodel. Similarly to the inputs, the output variables for the metamodel are identified. The simulation outputs measure the performance of the simulated system and they can be either discrete or continuous. Reflecting to the contributions of the Dissertation, in the construction of DBN and ID metamodels, the simulation output is a time series representing the state of the simulation model during the simulation which has not been studied in the existing literature. The problem structuring also specifies the validity measures used in validation of the metamodel. The *metamodel specification* refers to the selection of the type of metamodel. The type depends on, e.g., the characteristics of the simulation inputs and outputs as well as the goals of the analysis.

The *simulation experiment* consists of the experimental design and the collection of simulation data. The experimental design determines the values of the simulation inputs for which simulation runs are performed as well as the necessary number of simulation runs. The simulations are performed and the resulting values of the simulation outputs are collected into a simulation data set. In the *metamodel construction*, the metamodel is fitted to the simulation data by, e.g., estimating the values of its parameters. Finally, in *validation*, it is ascertained that the metamodel gives a good representation for the simulation model. Here, independent simulation data, cross-validation, or bootstrapping can be employed (e.g., Kleijnen 1998; Kleijnen and Sargent 2000; dos Santos and Porta Nova 2006; Kleijnen and Deflandre 2006; dos Santos and dos Santos 2010).

3.3 Approaches to Simulation Metamodeling

The most commonly used metamodels are input-output mappings that project the values of the simulation inputs to the expected values of the simulation output. Examples of such simulation metamodels are:

- Polynomial regression (Blanning 1974; Kleijnen 1979; Hopmans and Kleijnen 1980; Friedman 1984, 1989; Porta Nova and Wilson 1989; McHaney and Douglas 1997; Cheng 1999; Kleijnen and Sargent 2000; Tunali and Batmaz 2000, 2003; Kleijnen et al. 2001; Batmaz and Tunali 2003; dos Santos and dos Santos 2007, 2010)
- Non-linear regression (dos Santos and Porta Nova 1999; Kleijnen et al. 2001; dos Santos and Porta Nova 2005, 2006; dos Santos 2009)
- Kriging or spatial correlation (Sacks et al. 1989; Currin et al. 1991; Handcock and Stein 1993; Morris et al. 1993; van Beers and Kleijnen 2003; Staum 2009; Kleijnen 2009; Ankenman et al. 2010; Kleijnen et al. 2010)
- Radial basis functions (Hussain et al. 2002; Shin et al. 2002; Mullur and Messac 2006)
- Neural networks (Fishwick 1989; Hurrion 1992; Pierreval and Huntsinger 1992; Pierreval 1996; Badiru and Sieger 1998; Fonseca and Navaresse 2002; Fonseca et al. 2003; Wang 2005; Zobel and Keeling 2008; Yang 2010)
- Splines (Friedman 1991; Barton 1998; Keys and Rees 2004; dos Santos 2010)
- Response surface methodology (Biles 1974; Anjum et al. 1997; Barton 1998; Greenwood et al. 1998; Kleijnen and Sargent 2000; Batmaz and Tunali 2003; Myers et al. 2004; Barton and Meckesheimer 2006; Myers et al. 2009)

This list is not comprehensive and there exist also other types of simulation metamodels such as frequency domain models (Schruben and Cogliano 1987; Morrice and Schruben 1993; Arsham 1998; Morrice and Schruben 2001), fuzzy models (Madu 1995; Huber et al. 1996), and rule-based metamodels (Pierreval 1992). Reviews of various simulation metamodeling approaches can be found in, e.g., (Barton 1992, 1994, 1998).

The suitable type of metamodel depends on the objectives of the simulation study and other background information related to the system at hand (Cheng 2008). Polynomial regression models are used for local approximation of stochastic simulation outputs (Barton 2008).

Linear or quadratic models are often used as they offer a simple approach to simulation metamodeling and, moreover, they are transparent, i.e., the effects of individual simulation inputs and their interactions are easily interpretable. Therefore, they are the most popular simulation metamodels (Kleijnen 2008). In fact, Jin et al. (2001) proposes that when constructing a simulation metamodel, polynomial regression should be implemented first to check if a reasonable fit is obtained. If appropriate background information is available, phenomenon specific non-linear regression models can be used. Unfortunately, polynomial regression models are not applicable for global approximation as they may behave erratically in larger regions.

Global approximations for deterministic or stochastic simulation outputs are attained using Kriging models known also as spatial correlation models, neural networks, or splines (Barton 2008). Metamodels based on deterministic Kriging (Krige 1951) are sensitive to noise because they match the data exactly, i.e., over-fit to the noise (Jin et al. 2001). This issue is handled in stochastic Kriging by allowing for random variation in simulation outputs (Ankenman et al. 2010). Overall, Kriging models are flexible and give a good global fit. However, the effects of individual inputs on the output cannot be readily determined using Kriging models.

Some of the techniques, e.g., regression and Kriging models, involve assumptions about probability distributions of random factors included in simulation. Based on these assumptions, one can derive the probability distribution of the predicted output and present its confidence interval, in addition to the point estimates, which gives information about the accuracy of predictions. On the other hand, if the probability assumptions are not met, the prediction given by such models may be inaccurate or biased.

Radial basis functions and other neural networks, such as multi-layered perceptrons, are also used for the global approximation of outputs (Barton 2008). Similarly to regression models, neural networks accommodate the combination of continuous and discrete variables. Most neural network models are global, i.e., a single neural network is developed to represent the entire experimental region. This differs from polynomial regression metamodeling, where regression models are fitted to represent only subsets of the experimental region. Additionally, neural networks are not sensitive to deviations from traditional assumptions (Kilmer et al. 1999). This property makes them applicable to a wider range of simulation models but the accuracy of predictions for the outputs cannot be directly assessed by using, e.g., confidence intervals. This limitation can be avoided by constructing a parallel model for the variation of the simulation output and using it to calculate the necessary confidence intervals (Kilmer et al. 1999).

Spline based simulation metamodels are used widely for the approximation of deterministic simulation outputs (Barton 1998). The univariate splines can be categorized into three classes based on the tradeoff between smoothness and fitting the data. There are smoothing splines, interpolation splines, and regression splines. For simulation metamodels with multiple inputs, tensor products of univariate splines can be used (de Boor 2001) but such models require high number of simulation runs. Therefore, several alternative multivariate spline models have been proposed. For example, multivariate adaptive regression splines (Friedman 1991), produce accurate global approximations for deterministic outputs with reasonable computational cost. Unfortunately, such models perform poorly for small sample sizes (Jin et al. 2001).

The methodology of response surfaces (see, e.g., Myers et al. 2009) refers to simulation metamodeling where sequential experimental designs are combined with other metamodeling techniques in order to optimize the values of simulation outputs. In practice, a series of local metamodels such as regression models (Kleijnen and Sargent 2000) are fitted to simulation data as the optimization progresses. In the case of metamodels that can provide global fit, e.g, neural networks (Anjum et al. 1997), a global model can be fitted once at the beginning of the optimization, or the model can be refined based on the additional information acquired during the optimization.

The existing simulation metamodels discussed above are static input-output mappings. For many of the goals presented in Table 1, this is sufficient but such models do not explicitly present the time evolution of the simulation which may provide valuable information about the system under consideration. The Dissertation tackles this limitation by introducing metamodels based on the methodology of Bayesian networks and influence diagrams that describe the progress of the simulation and depict the probabilistic dependence between the simulation state variables at different time instants.

One of the goals of simulation metamodeling pointed out in Table 1 is simulation optimization. Many iterative optimization methods are designed for deterministic optimization problems and, therefore, they cannot be directly applied to settings when the system performance is evaluated by stochastic simulations. Therefore, various metamodels have been used in optimization in order to convert the stochastic optimization problem into a deterministic one and expedite the necessary computations (Barton and Meckesheimer 2006; Barton 2009; Kleijnen et al. 2010). A comparison of metamodeling techniques in simulation based optimization is given by (Li et al. 2010). Simulation metamodels have also been applied to multi-objective optimization (Yang and Chou 2005; Rosen et al. 2008; Zakerifar et al. 2009) but so far only simulation settings with a single decision maker, i.e., settings where the decision maker controls all the simulation inputs, have been discussed. This is a limitation that excludes the application of simulation optimization in game settings representing conflict situations involving multiple decision makers such as air combat. With the game theoretic metamodels introduced in the Dissertation, such studies can be conducted. The contributions of the Dissertation are discussed in more detail in the following section.

4 The Dissertation

The Dissertation introduces simulation metamodeling techniques from the viewpoint of novel perspectives reflecting time and conflict. The first perspective is covered by Papers [I]-[IV] that present how the time evolution of discrete event simulation (DES) is effectively and efficiently described using dynamic Bayesian networks (DBNs) and influence diagrams (IDs). With respect to the conflict perspective, the game theoretic metamodeling approach covered by Papers [V]-[VI] enables the application of existing metamodeling techniques to simulation studies of game settings in which multiple decision makers interact and try to direct the system into a state that matches their own objectives. The contribution of the Dissertation is summarized in Table 2. In the following, the contributions of the individual papers are specified in greater detail.

Table 2: The Papers.

Paper	Context	Methodology	The Contribution
[I]	Study of time evolution of discrete event simulation	Dynamic Bayesian networks	Discrete time DBN metamodel for the time evolution of simulation enabling the calculation of marginal and conditional probability distributions of simulation state variables
[II]	Study of time evolution of discrete event simulation in continuous time	Dynamic Bayesian networks and interpolation	Extension of DBN metamodel into continuous time using first-order Lagrange interpolating polynomials
[III]	Study of time evolution of air combat simulation	Dynamic Bayesian networks	Application of DBN metamodel into a real-world air combat simulation problem
[IV]	Simulation based decision making and optimization	Influence diagrams	ID metamodel describing the consequences of decision alternatives and enabling the solution of optimal decisions
[V]	Simulation based decision making and optimization in settings involving multiple decision makers with conflicting objectives	Game theory, analysis of variance, and regression analysis	Game theoretic metamodels for analyzing decision makers' best responses and resulting equilibrium solutions
[VI]	Simulation based decision making and optimization in settings involving multiple decision makers with conflicting objectives	Game theory and stochastic Kriging	Extension of game theoretic metamodels using stochastic Kriging which results in globally applicable payoff functions

Paper [I] introduces a metamodeling technique for analyzing the time evolution of DES with DBNs (Pearl 1986; Dean and Kanazawa 1990; Neapolitan 2004; Jensen and Nielsen 2007). The paper gives guidelines for the construction of DBN metamodels from simulation data together with expert knowledge. The DBN metamodel consists of chance nodes representing random variables, their interconnecting arcs, and conditional probability tables that define the joint probability distribution of the random variables. The random variables represent the simulation state variables at discrete time instants, viz., the time slices of the DBN, whose number and positioning is determined in the construction of the metamodel. The optimal time instants of the time slices are found by solving an optimization problem where the approximation error between the model and the simulation data is minimized. The approximation error is defined as the maximum absolute difference between probabilities estimated directly from the data and a piecewise linear interpolation based on the probabilities given by the DBN. The resulting non-convex and non-linear optimization problem is solved using a genetic algorithm (Goldberg 1989).

After the variables and the time instants have been selected, the structure of the DBN, i.e., the arcs connecting its nodes, is determined in two steps. An initial network structure showing the obvious dependencies between simulation state variables is outlined by an expert. Then, the simulation data are searched for additional statistically significant dependencies using, e.g., the greedy thinning algorithm (Heckerman 1995). When the structure of the DBN has been determined, the conditional probability tables are estimated from the simulation data using the maximum likelihood estimators for the probabilities of multinomial distribution (Heckerman 1995), i.e., the relative frequencies of the combinations of the values of the variables are calculated. In practice, the construction and use of DBN metamodels is performed using software designed for the analysis of Bayesian networks (BNs) such as GeNIe (Decision Systems Laboratory 2010).

The DBN is used to calculate marginal and conditional probability distributions of the simulation state variables as function of time. In what-if analysis, the value of the simulation state at a one of the time instants included in the model is fixed and the probability distributions of the state variables at other time instants are updated using the DBN which is faster and more effortless than the estimation of these distributions from raw simulation data. For these purposes, there exist numerous exact and approximative inference algorithms (e.g., Neapolitan 2004; Jensen and Nielsen 2007). In all the examples presented in this Dissertation, the updating is performed using the clustering algorithm (e.g., Lauritzen and Spiegelhalter 1988) that is an exact inference algorithm readily implemented in GeNIe.

Simulation input variables can also be included in the DBN as random variables in order to describe the dependence between the values of the inputs and the evolution of the simulation. Furthermore, the inputs can be treated as uncertain factors and the effect of this uncertainty on the simulation can be studied. The accuracy of the estimates of probabilities and expected values produced by the DBN is assessed by calculating appropriate confidence intervals. It is important to note that DBN metamodels differ from the more traditional simulation metamodels, e.g., regression models and neural networks, in the sense that they are not used to predict simulation outputs for values of inputs that are not included in the experimental design. Instead, the DBN metamodels are used to describe the progression of simulation runs for the design sites for which simulations have already been performed, i.e., the design sites of the simulation experiment.

Paper [II] presents an approximation scheme that extends the above mentioned DBN metamodels into continuous time. In Paper [I], the positioning of the time slices of the DBN metamodel is determined during its construction and the following analysis is limited to these discrete time instants. This limitation could be alleviated by including more time slices into the DBN. However, each additional time slice increases the size of the DBN. This is undesirable as the effective size of the model and the computational effort needed in its analysis depend on, e.g., the number of state variables, the number of their states, and the number of arcs in the network – even though there exists no clear upper limit to the number of nodes included in the DBN. In Paper [II], the need for additional time slices is circumvented by introducing an interpolation scheme that utilizes probability estimates produced by a DBN metamodel. The scheme yields approximative probability distributions representing the simulation state at any given time instant using first-order Lagrange interpolating polynomials. This allows one to conduct analyses similar to those presented in Paper [I] without limitations to the time instants.

Paper [III] presents a case study where a DBN metamodel is utilized in analysis of air combat simulation model called X-Brawler. The paper gives a real-life application of a DBN metamodel where it is used to effectively communicate the progress of the simulation and conduct highly detailed what-if analyses. One should note that Papers [I]-[II] also include similar examples related to air combat. However, in those examples the simulation state represents only the pilot being alive or dead, while in Paper [III], the state of the simulation is determined by the actions of the simulated pilots. In X-Brawler, these actions are controlled by the pilots' mental models that describe their perception of the phase of the air combat and situational awareness. For example, at a given time a simulated pilot can be attacking the opponent or evading a missile launched by the opponent. In the case study, the simulation state is defined based on the phases of the pilots and the progress of the air combat is represented by the changes in the probability distribution of the simulation state. In comparison with the examples presented in Papers [I]-[II], it is seen that the alternative representation of the simulation state leads to different potential analyses. That is, the richer state space enables more detailed analysis, e.g., how the actions of the pilots affect their survival probabilities.

In Paper [IV], influence diagrams (Howard and Matheson 1984, 2005), which have been widely used in structuring and solving decision problems under uncertainty, are introduced as simulation metamodels. The paper expands the descriptive analysis discussed in Papers [I]-[III] to simulation based decision making and optimization by constructing influence diagrams from simulation data. In practice, the ID metamodels are DBNs with additional nodes representing the decisions and objectives of the decision maker. In the construction of an ID metamodel, a DBN is first built to present the evolution of the simulation state. Then, the input variables of the simulation model are represented by the decision nodes of the network. The preferences of the decision maker are included by adding a utility node and a corresponding utility function (von Neumann and Morgenstern 1944). The utility function is defined as a function of the simulation output and it measures the attainment of the objectives of the decision maker. The constructed ID is then solved to find the optimal decision alternatives that maximize the expected value of the utility function. The paper gives two example analyses. In the first example, a DBN metamodel is used to describe the behavior of an aircraft maintenance simulation model (Mattila et al. 2008). In the second example, a decision problem related to simulated air combat is studied using an ID metamodel.

Paper [V] introduces the game theoretic approach to simulation metamodeling where game theory (e.g., Fudenberg and Tirole 1991; Başar and Olsder 1995) is applied to the analysis of systems and corresponding simulation models related to game settings, i.e., decision problems with several decision makers called players, pursuing their own objectives. The game theoretic metamodels, like game models in general, consist of players as well as their decision variables and payoffs. Decision alternatives available to the players are presented by the ranges of the decision variables. The payoffs depend on the decision variables and evaluate the attainment of the players' objectives. The outcome of the game, i.e., the values of the players' payoffs, is determined based on the decision alternatives selected by the players.

Paper [V] presents the construction procedures for game theoretic metamodels involving discrete or continuous decision variables. In the discrete case, analysis of variance (e.g., Montgomery 2001) is applied to classify the values of the simulation outputs into payoffs that are collected to a matrix form game. With continuous variables, a multivariate regression model (e.g., Milton and Arnold 1986; Sharma 1996) is fitted to the simulation data yielding the payoffs of the players. By using the game theoretic metamodels in simulation analysis, one can identify the players' best responses to the opponents' decisions, i.e., the game optimal value of the player's decision variable when the action of the opponent is fixed. Together, the players' best responses determine the equilibrium solutions of the game, e.g., its Nash equilibria. The constructed game theoretic metamodels are applicable both for validation of simulation models as well as for comparison of decision alternatives in game settings.

Paper [VI] combines the game theoretic approach with stochastic Kriging (Ankenman et al. 2010). In this paper, the payoffs of the players are constructed with stochastic Kriging yielding simulation metamodels that offer a global fit to the simulation data. On the other hand, the paper introduces so called best response and Nash equilibrium sets to simulation metamodeling. The players' best response sets are used to tackle the effects of the random variation included in the estimates of the players' payoffs. These sets consist of the values of decision variables that produce a payoff that is close to the optimal solution, i.e., does not differ statistically significantly from the best response. The intersection of the best response sets forms the Nash equilibrium set of the game. Furthermore, Paper [VI] demonstrates how the game theoretic approach can be applied to any type of simulation metamodel listed in Section 3.3.

In addition to the new analysis capabilities, the novel techniques discussed above can also be used to pursue most of the recognized goals of simulation metamodeling listed in Table 1 which is shown in Table 3. From the system perspective, all the presented techniques increase the understanding over the system under consideration and allow the testing of hypotheses related to it. The results obtained with the new metamodels could be generalized to other similar systems but this aspect has not been explored in the Dissertation.

In the air combat case study presented in Paper [III], a DBN metamodel reveals the progress of the simulation by carefully describing the action of the simulated pilots. Addi-

Table 3: Applicability of the metamodeling techiniques presented in the Dissertation.

Goal	Paper					
	[I]	[II]	[III]	[IV]	[V]	[VI]
System perspective						
Understanding the behavior of the system	*	*	*	*	*	*
Hypotheses testing	*	*	*	*	*	*
Generalization to other systems						
Simulation perspective						
Simplification of the simulation model	*	*	*	*	*	*
Interpretation of the simulation model	*	*	*	*	*	*
Verification and validation of the simulation model			*		*	*
Input-output perspective						
Prediction of outputs					*	*
Sensitivity analysis	*	*	*	*	*	*
What-if analysis	*	*	*	*	*	*
Inverse questions	*				*	*
Optimization of outputs				*	*	*
New capabilities						
Time evolution of simulation	*	*	*	*		
Consequences of decisions				*		
Analysis of conflict situations					*	*

tionally, the game theoretic approach is particularly well-suited for validation of simulation models as it allows elaborate analysis of simulation outputs and the consequences of the decision makers' game optimal decisions.

From the input-output perspective, DBN and ID metamodels can be used for sensitivity and what-if analyses. The DBN metamodels that include simulation parameters as random variables, as discussed in Paper [I], are also applicable for the study of some inverse questions. The ID metamodels introduced in Paper [IV], on the other hand, are intended for optimization of simulation inputs. The game theoretic metamodels dealing with continuous simulation inputs are an example of prediction of simulation outputs because the payoffs are given for all possible combinations of the simulation inputs. The analysis of the players' best responses can be interpreted as any of the alternatives listed under the input-output perspective, i.e., sensitivity analysis, what-if analysis, inverse questions, and optimization of outputs.

To summarize, the techniques introduced in the Dissertation enhance the existing simulation metamodeling techniques in ways that are particularly relevant to air combat simulation but can be applied to any simulation models. First, the time evolution of DES models is studied using DBNs and IDs. Second, the game theoretic approach to simulation metamodeling offers an extension of simulation based decision making and optimization to analysis of conflict situations with multiple decision makers. This includes all military simulations but also other simulations describing game settings.

5 Conclusions and Future Research Directions

The Dissertation introduces the utilization of dynamic Bayesian networks, influence diagrams, and games in simulation metamodeling. The presented techniques offer new analysis capabilities to simulation analyses that are beyond the scope of existing simulation metamodels. The DBNs and the IDs are useful in the analysis of time dependent systems while games are used in the analysis of conflict situations.

The existing simulation metamodeling techniques do not exploit the dynamic and temporal properties of DES but stunt the simulation into a static input-output mapping. The progress of the simulation can be visualized, e.g., with animations. However, a human analyst cannot digest animations of hundreds or even thousands simulation runs in order to summarize the relevant features of the time evolution of the system. The DBN and ID metamodels assemble the simulation data into a probabilistic narrative of the time evolution of the simulation. Furthermore, what-if analyses enabled by the DBN metamodels reveal the consequences of fixed simulation states in terms of resulting simulation states. Thus, the DBNs do not only present a dynamic sequence of changes in the simulation state but also give a representation of causes and effects.

The analysis of cause and effect is extended further by the ID metamodels. When ID metamodels are utilized in the optimization of the simulation output, they also describe the consequences of the decision alternatives, i.e., the time evolution of the simulation conditional on the chosen alternative. Thus, the ID metamodels are used, in addition to the optimization, to better understand what actually happens during the simulation.

The game theoretic approach expands the use of simulation based optimization to the study of conflict situations. By constructing games based on simulation data and using them in the optimization of simulation outputs, the existing techniques for simulation optimization are extended into a two-sided setting as the joint effects of the sides' decisions are taken into account – instead of unilateral optimization. This capability is crucial, e.g., in air combat simulation analyses as well as in other military applications of simulation.

In the future, DBN metamodels similar to those introduced in Papers [I]-[III] could be used as a part of a Bayesian network (BN) that is constructed using, e.g., expert knowledge, to represent a larger system or a system of systems. For example, air combat simulation results can be included in Bayesian networks used as a tool in planning of effects-based operations (Pousi 2009). Alternatively, simulation data produced by several simulation models could be integrated using BNs, DBNs, or IDs in order to describe interdependencies between systems. For example, the results produced by simulations of air combat and maintenance of aircraft (Mattila et al. 2008) could be combined for a more comprehensive representation of air operations.

The DBN metamodels include random variables corresponding to simulation inputs that are time invariant. These variables could also depend on time representing, e.g., changes in the system environment. Also, in the presented DBN metamodels, all simulation state variables are depicted at common time instants, i.e., all the state variables are included in all the time slices. An alternative would be to associate each simulation state variable with its own time instants and time slices in the DBN. In this way, state changes taking place with different rates could be treated more effectively. Additionally, BNs could be utilized in simulation metamodeling as more traditional, static input-output mappings. Such models could be used as non-parametric simulation metamodels, i.e., without any assumptions about the functional form of the probability distributions, for the uncertainty related simulation inputs and the interdependencies between simulation outputs (Poropudas et al. 2011a).

Thus far, simulation studies using DBN metamodels have been performed with software designed for the analysis of BNs such as GeNIe (Decision Systems Laboratory 2010) or HUGIN (Andersen et al. 1990). The optimal selection of time instants presented in Paper [I] and the multivariate interpolation used in the continuous time extension presented in Paper [II] are beyond the scope of such software and thus these tasks have been performed, e.g., on MATLAB (Mathworks 2011). In order to promote and aid future studies, it might be worthwhile to develop an automated tool designed for the construction and utilization of DBN metamodels together with the multivariate interpolation.

The ID metamodels discussed in Paper [IV] involve decision problems with a single objective. The single-criterion view could be broadened to problems related to multi-criteria optimization and decision making (e.g., von Winterfeldt and Edwards 1986; Ehrgott 2005) by utilizing multi-criteria IDs (MCIDs, Diehl and Haimes 2004) as simulation metamodels. The MCID simulation metamodels would give a non-parametric multiple-input multiple-output (MIMO) model for simulation data (Poropudas et al. 2011a,b). Such MIMO metamodels could present the joint probability distribution of simulation inputs and outputs, unlike existing MIMO metamodels (e.g., Friedman 1989; Porta Nova and Wilson 1989; Charnes 1995; Myers et al. 2004) that limit the analysis to the expected values of simulation outputs. The MCID metamodels could be used for various what-if analyses as well as for efficient solution of optimal and/or non-dominated decision alternatives. Furthermore, the ID metamodels presented in Paper [IV] only discuss decision problems with discrete decision variables. This limitation could be answered using a similar interpolation scheme as in Paper [II]. That is, approximate solutions for problems with continuous decision variables could be achieved by the application of discretization and interpolation to the revelant variables.

The game theoretic approach to simulation metamodeling introduced in Paper [V] offers numerous possibilities for future research. One potential topic is the so called "games against nature" (e.g., Webb 2006), i.e., games where one of the players is a virtual decision maker called nature. Such games could be used in simulation based decision making, e.g., to assess the potential consequences of uncertainties and to consider the worst possible outcomes of decisions (e.g., Başar and Olsder 1995). With such an extension, game theoretic simulation metamodels could be utilized in the analysis of almost any stochastic simulation model – including those without an inherent game setting. On the other hand, other types of simulation metamodels discussed in Section 3 could be used as basis for game theoretic simulation metamodels. This is demonstrated in Paper [VI] where stochastic Kriging is applied.

Paper [V] discusses only the most elementary concepts of game theory in context of simulation metamodeling which could be developed further by considering alternative game formulations. For example, only pure strategies (e.g., Fudenberg and Tirole 1991) are used, i.e., the players have to select one of the available decision alternatives. The game theoretic metamodels could also allow the players to employ mixed strategies (e.g., Fudenberg and Tirole 1991) where their decisions are represented by probability distributions over the available alternatives. On the other hand, the application of game theory to the ID metamodels would result in influence diagram games (Koller and Milch 2003), i.e., IDs with multiple decision makers, as game theoretic simulation metamodels.

The ID metamodels could also be applied to the construction of multi-stage influence diagrams representing a sequence of decisions. This kind of ID has been used in analysis of air combat (Virtanen et al. 2004) but the models have been constructed based on expert analysis – instead of simulation data. Influence diagram games representing air combat (Virtanen et al. 2006) could also be constructed from simulation data. Another potential application area for the game theoretic approach is virtual simulation, i.e., simulation where real pilots fly operations in simulated environments. Thus far, the simulation studies have been mainly based on constructive simulations but similar analyses could be conducted by constructing metamodels from simulation data based on virtual simulations as well.

The novel perspectives to simulation metamodeling presented in the Dissertation allow the inclusion of time evolution and conflict situations into simulation analyses. The DBN and ID metamodels offer a transparent narrative for the progress of simulation and its internal dependencies. The game theoretic approach, on the other hand, can be incorporated with any other simulation metamodeling technique in order to study game settings. Although, many of the examples presented in the Dissertation concentrate on simulation of air combat, the new metamodeling techniques are not limited to military applications. The DBNs and the IDs can be applied to all DES models. Similarly, at least with the extension to games against nature, games can be constructed based on any stochastic simulation data. Overall, the metamodeling techniques innovated in the Dissertation are a valuable addition to the already rich field of simulation metamodeling because they enable even more informative and flexible simulation analyses.

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