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Comparative Modelling and Simulation

A Concept for Modular Modelling and Hybrid Simulation of Complex Systems

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Kurzfassung

Basierend auf etablierten Methoden der Modellbildung & Simulation wird in dieser Arbeit ein Konzept zur Erweiterung des Modellierungsprozesses, sowie zur Analyse, Bewertung und Vergleich verschiedener Strategien bei der Umsetzung von Simulationsprojekten erarbeitet und vorgestellt. Darüber hinaus werden anwendungsbasierte Konzepte zur Umsetzung, Verbesserung und Erweiterung des gesamten Simulationsprozesses vorgestellt.

Methoden wie Differentialgleichungen, Agent Based Modelling, zelluläre Automaten, System Dynamics, Markov-Modelle oder diskrete Modelle werden bezüglich qualitativer und quantitativer Unterschiede und Äquivalenz untersucht und verglichen. Dabei werden in Vergleichsstudien prinzipielle Unterschiede herausgearbeitet bzw. „Cases" definiert, wann Modelle nicht mehr äquivalent dargestellt werden können. Dies geschieht mit dem Fokus auf die unterschiedlichen Einzelschritte in der Umsetzung einer konkreten mathematischen bzw. modelltechnischen Fragestellung.

Eine Grundannahme der Arbeit ist dabei die Hypothese, dass unterschiedliche Modellierungsmethoden für ein System bzw. einen Prozess existieren, diese voneinander unterscheidbar und vergleichbar sind und diese Differenzierung nach der Definition des Modellierungsprozesses sinnvoll ist. Dieser Gedanke wird dabei nicht nur auf das zu modellierende Gesamtsystem, sondern auch auf Teilsysteme- und Prozesse in einer geschlossenen, dynamischen Simulation angewendet. Darauf aufbauend wird gezeigt, dass die daraus resultierende Herausforderung der Auswahl der geeigneten Methode idealer Weise nicht methodengetrieben, sondern daten- bzw. strukturgetrieben ist und immer abhängig von der Forschungsfrage sein sollte.

Notwendig werden diese Überlegungen durch das oftmalige Erreichen der Machbarkeitsgrenzen der Simulation von Modellen in der Praxis, die heute oft steife, hyperkomplexe, nicht homogene und schwer zu parametrisierende Systeme darstellen. Sei es im technischen Bereich, etwa im Bereich komplexer Infrastrukturvorhaben, wo unterschiedliche Systeme (Thermodynamik, Elektronik, Mechanik) oder Systeme mit stark unterschiedlichem Skalenniveau zu verkoppeln sind, oder im Bereich komplexer Entscheidungsprozesse im Gesundheitssystem, wo komplexe Datenstrukturen und schwierig zu definierende Zielfunktionen in ein geschlossenes Modell umzusetzen sind. Diese Probleme und mögliche Lösungen werden mittels unterschiedlicher Beispiele dargestellt und beinhalten neben den Problemstellungen die Präsentation unterschiedlicher Lösungsansätze.

Im speziellen werden modulare Modelle und hybride Simulationskopplungen betrachtet, unterschiedliche Modelle werden quantitativ und analytisch auf ihre Äquivalenz untersucht. Schrittweise werden so die Grenzen unterschiedlicher Darstellungsweisen eines Modells dargestellt.

Zu guter Letzt werden die Konzepte „Falsifikation“ und „Cross Model Validation“ als Beispiele für die neuen Möglichkeiten im erweiterten Modellierungsprozess präsentiert, sowie Beispiele der Anwendung der erzielten Ergebnisse in Forschungsprojekten zu komplexen Systemen.

Abstract

Based on established methods of modelling & simulation, a concept for an extension of the modelling process, as well as to analyse, evaluate and compare various strategies in the implementation of simulation projects is developed and presented in this work. In addition application based concepts for implementation, improvement and extension of the whole simulation process are described.

Methods such as differential equations, Agent Based Modelling, cellular automata, System Dynamics, Markov models or discrete models are examined and compared for both qualitative and quantitative differences and equivalence. Fundamental differences are identified in comparative studies and "cases" will be defined when models cannot be represented in an equivalent way. This is done with the focus on the different individual steps in the implementation of a specific mathematical model or model theoretical question.

One basic assumption of the work is the hypothesis that different modelling methods for a system or a process exist, they are distinguishable from each other and comparable, and this differentiation is useful according to the definition of the modelling process. This idea is thereby applies not only to the overall system to be modelled, but also on subsystems and sub processes in a closed, dynamic simulation. Based on this, it is shown that the resulting task of the selection of the appropriate method ideally should not be driven by methods, but depends on system data, system structure and - knowledge and the research questions given.

These considerations are necessary as often the feasibility limits of classical, "state of the art" simulation models comes to an end, as in practice today often rigid, hyper-complex, non-homogeneous and difficult to parametrise systems have to be modelled. For example in engineering we can assume the analysis of complex systems in functional infrastructure. Here different systems (thermodynamics, electronics and mechanics) or systems with highly different scale level have to be coupled. Or in complex decision making in health systems, where complex data structures and complex research questions and objectives have to be implemented in a closed model. Arising problems and possible solutions are presented in this work with various examples. The work is not only focused on remarks on boundaries of methods, but also focuses on the responsibility of the user/developer in the modelling process to define system limits and what tools are needed for doing so.

In particular modular modelling and hybrid simulation couplings are considered different models are examined stochastic or analytically on their equivalence. Gradually the boundaries of different representations of a model are shown. The

work concludes with presentation of the concepts of "falsification" and "cross model validation" as examples for resulting possibilities of the extended modelling process and applications of our work in research projects on complex systems.

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Und ich bedanke mich bei Helene Breitenecker.

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Contents

1 Introduction - Examples & Motivation

"The greatest danger in times of turbulence is not the turbulence;
it is to act with yesterday's logic."

Peter Drucker

The presented work deals with „Comparative Modelling". But what do we mean by „Comparative Modelling"? And why do we need to deal with it? The basic idea is that in an ideal world there is a closed model theory. As a result all possible systems (see definition below) or at least problems (well defined research question within a given system) can be modelled within one closed theory. This would have a lot of benefits, as all models could be classified, compared and combined. So one would always know (or at least would be able to know) how to choose the right model and which model is the best choice. Additionally in the case of the extension of system boundaries or the case of re definition of the problem, the extension of the model to fit to the new challenge would be easy and consistent.

Unfortunately we don´t have and probably can´t get a general theory of modelling and simulation. As the world is complex and depending on the „segment" of the world (the so called domain) we have to look at, we can measure different things (experiment) and find different characteristics, feedback loops and interdependencies of the system (theory). So depending on the different domains we have different possibilities of gaining knowledge of the system. As a result we probably need different characteristics for model concepts describing this domain. But at least in modelling & simulation different formal approaches have been developed over the last decades.

As we will see depending on the point of view these differences are not (only) an effect of the approach we select, but the differences can be assumed as „system immanent", following the ideas of sociologist Niklas Luhmann. So even if we want to, we could maybe not change these concepts easily in our models. The question which arises is: how can we nevertheless compare models and what is it good for?

Breitenecker and Troch wrote in (Unbehauen, 2009): *„A 'simulation' is a method for solving a problem in dynamical systems, which investigates instead of the real system a model of the system."* Steps for doing a simulation are *„ (1) formulation of the problem,* *(2) data collection, (3) mathematical modelling, (4) computer implementation, (5) model validation, (6) model identification, (7) experiments with the model, (8) representation of results, and (9) interpretation of results."* (Unbehauen, 2009). As mentioned above characteristics of systems in different domains differ, and so the mentioned steps also do. We can see a summary of this idea in the figure below:

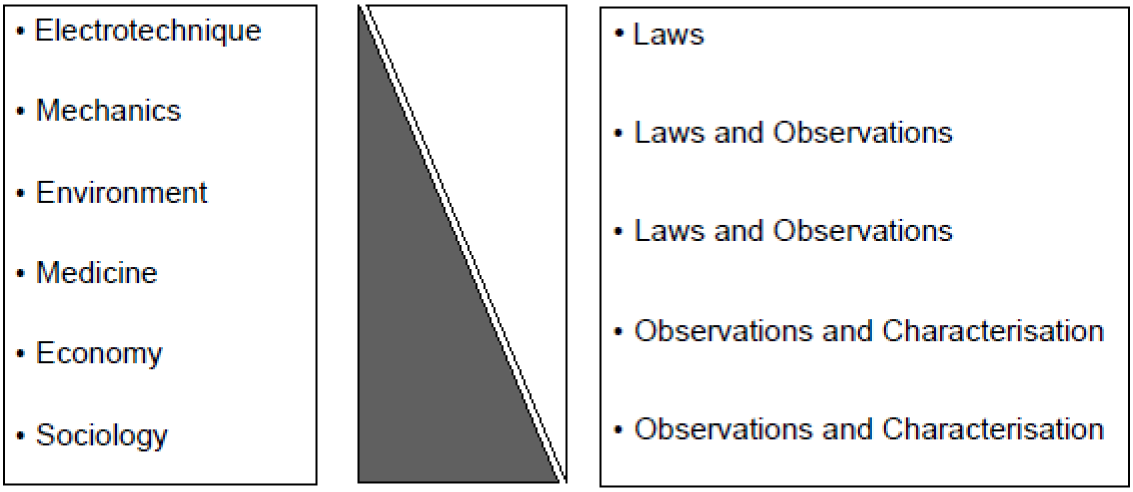


Figure 1.1: Basis for Model Development in Different Domains

„White Box"-Modelling is applicable in domains, where we can rely on laws and observations. Stepwise we come in other domains to the „Black Box"-Modelling concept, where we can only rely on Observations and even more on Characterisation of the systems. As we will see this is not a sign of „quality" in terms of „how good is the theory" in this domain, but a difference of domains in terms of what is the domain immanent knowledge we can use to build a model and a simulation.

Finally at least we have different formalisations and classifications for models and simulations especially for the steps (1),(2),(3),(5) and (6) and (9) of the process mentioned above. Different domains allow different approaches and they are shaping the set of mind in the domains and the mentioned process steps. This leads us to today's situation, that in various domains we have very different approaches of describing models for the problems. A lot of good approaches exist to describe the various needs, as we can see the world continuous or discrete, deterministic or stochastic, top-down or bottom-up and so on. Additional as a matter of fact we have - in a wide area - very different formal settings, where we use mathematical skills for generating PDE models use control theory for engineering, system theory for biology or sociology or Markov chains for clinical models in medicine and many more.

Nevertheless an exchange could be synergetic, as we can assume, that knowledge is available in different domains, which could be used in other domains, e.g. analysis of data sets, modelling of similar processes and many more. As a matter of fact the potential is growing. The author worked for several years as CEO of a small simulation company for projects in various application areas and domains. In industry, project management, architecture different tools try to solve different application or domain immanent problems. The foundations of these theories are based in different research areas like informatics, mathematics or network theory. They have in common, that they are not sufficient in solving the tackled questions any more, as the systems become bigger and more complex.

So we are at the point, where we have well defined concepts for modelling & simulation in various domains, but the systems we have to deal are becoming bigger. Research questions are more sophisticated and last but not least we get huge streams of data every second, ready for parametrising our models.

The idea of this work is, that based on a more or less general understanding of system theory and system simulation we admit that there is, as described, no „unified theory“ for modelling real world problems. In this work we try to define some additional ideas to categorise existing concepts, how to improve the possibilities to compare, combine and couple those efforts and how to improve the general simulation processes a little. The mentioned concepts and examples in this work are a summary of recent and actual work of our research group and last but least gives an outline of the work in the near future. Among these ideas is the analysis of Agents Based concepts and their relation to Markov chains, transferable formal definitions of model concepts for future comparison and the analysis of boarders of these formal descriptions.

The idea of the presented work is (1) to give a general idea how model comparison can be improved. Improving the possibility to compare approaches, we improve our ability to combine them. Better combining potential leads us to the question when and how to combine and how to switch between them. In addition it will deal with (2) some examples for resulting approaches for detail questions like the concept for cross model validation of models, which improves the ability to separate system immanent and model immanent behaviour and improves the opportunity for validating models for complex systems and process. Last but not least (3) solutions for examples in big scaled projects in modelling and simulation from the areas complex functional infrastructure and complex decision making will be presented.

All this will be done with the focus on the modelling circle, the simulation pipeline and the concept, that those modelling and simulation concepts can be transferred between different application areas and domains.

1.1 Motivation from Domains

As mentioned above different domains and systems have different model concepts. In classical, technical applications they are well described (e.g. Fritzson, 2004; Cellier, 2006; Succi, 2001). For complex systems, like big infrastructures combined with dynamic, interacting processes or decision processes with human interaction we take a look at Niklas Luhmann's "Soziale Systeme: Grundriß einer allgemeinen Theorie" (Luhmann, 2012) to get an idea why this happens. Luhmann developed a system theory, where he focusses on social systems. The most important aspect of such systems is communication. For Luhmann a system is defined by a boundary between itself and its environment, dividing it from an infinitely complex and chaotic, exterior by communication. The interior of the system so becomes an area of reduced complexity (Luhmann, 2012).

Communication within a system operates by selecting only a limited amount of all information available outside. This process is also called "reduction of complexity". The criterion according to which information is selected and processed is meaning. Social systems operate by processing this meaning. Society is in Luhmanns point of view the most comprehensive social system. Being the social system that comprises all (and only) communication, today's society is a world society (Luhmann, 1982).

Definition 1.1 (System). A system ($\mathcal{S}$) is defined by a boundary between itself and its environment, dividing it from a complex and chaotic exterior (environment) by communication (resulting in relations). Subsystems ($\mathcal{S}_i$)can be defined analogue[1].

From the aspect of modelling & simulation the most interesting aspect is that from a technical point of view we could ask how subsystems contribute to the functioning of the system (e.g. the next higher system or overall society). As described above, Luhmann starts with the differentiation of the systems themselves out of a not described environment. He does observe how certain systems fulfill functions that contribute to "society" as a whole, but this is happening more or less by chance, without an overarching vision of society.

[1] From the point of view of the subsystem, it is not relevant, that outside the subsystem, the structure is well defined.

Each system has a distinctive identity that is constantly reproduced in its communication and depends on what is considered meaningful and what is not. If a system fails to maintain that identity, it ceases to exist as a system and dissolves back into the environment it emerged from. Luhmann called this process of reproduction from elements previously filtered from an over-complex environment autopoiesis which means self-creation, using a term coined in cognitive biology by Humberto Maturana and Francisco Varela (Maturana & Varela, 1980)

Luhmann likens the operation of autopoiesis (the filtering and processing of information from the environment) to a program, making a series of logical distinctions and differences, which Maturana and Varela had earlier identified as a model for the functioning of any cognitive process. The "self-creation" of any given system is an auto-referential process. Systems are continuously confronted with the dilemma of disintegration or continuation and selection or rejection.

Finally, the systems' autopoietic closure means that each system works strictly according to its very own code and has no understanding at all of the way other systems perceive their environment. For example, the economy is all about money, so there is no independent role in the economic system for extraneous aspects such as morals. This "code" means in Luhmanns sense, that every system develops its own language and formalisations.

Definition 1.2 (Model)**.** A triple with two systems and a surjective mapping f is a model. We have the object system, the model system, and f the model mapping.

As a result structures of systems are different not only by description of the system (a model), but already by the result of the process how they are built up. So we could never describe them "in a closed" way, as the different subsystems of society are different. As only a limited amount of all information available outside are selected for a system, to reach a "reduction of complexity", we have the basis for the concept of „formalisation" within a domain, as already the system itself is already reduced. The criterion according to which information is selected and processed is meaning, which we also will find again within the modelling process, when we define research questions within a domain or a system. According to Luhmann also for different subsystems of society different "languages" and words are used. In a technical point of view we use different modelling methods.

Definition 1.3 (Domain). A Domain is a system with common formalisms (f_i) for mapping (and describing entities and relations).

From now on we don´t want focus on the concept of autopoiesis further more, but we keep in mind, that it is not in our ability, simply to re-define the subsystems to make them comparable, which would be our first choice, as the system we have to model become now more complex, in the meaning, that systems which are not compatible have to be dealt with within one model & simulation project. As a matter of fact we have various problems to deal with in the practical world of simulation. Variation is from scheduling discrete processes in industrial applications to supporting decision making in health system research. Approaches are totally different in all cases and so are the methods. But today we can monitor a change. The systems are converging, as the systemic point of view broadens.

Two examples from the area of complex infrastructures and complex decision support problems will be presented, which will be analysed throughout the work:

- Complex Systems in Functional Infrastructure
- Complex Decision Processes in Health Systems

1.1.1 Complex Systems in Functional Infrastructure

Complex Systems in Functional Infrastructures are systems with complex internal processes in combination with a multi-layer infrastructure. These systems can be airports, railway stations, big markets or industrial production plants. They share an actual development, where intense changes in the processes are related with a huge increase if available data and changing boundaries. These might be cities, big infrastructures developments that may be seen as cities themselves or large buildings with infrastructure usually have a lot of processes going on within. Fort detailed descriptions we refer to the work of our group in (Bruckner, 2009; Emrich 2009; Emrich 2012; Bruckner, 2014)

These different processes are somehow connected to each other in ways that may not be so apparent at first. These large systems, broken into pieces, consist of different subsystems with much more detail. On the one hand the modeller looks at the system as a whole, decides which method suits best modelling the large system answering the research question. So in parts of the model of the large system the modeller has to make some trade-offs, where he can’t go too much into detail, where it would have been necessary or where he goes too much into detail, where it was not necessary. So with the model, the system may not be represented as realistic as it could have been. On the other side, when only modelling a small part of a large system with a specific modelling method and not taking into account effects from other subsystems the modeller again makes some trade-offs and propagated errors follow through the model. When different questions addressing for example the utilization of resources within one subsystem, or waiting times or even the planning process itself, arise, usually different modelling methods are used to model the specific subsystem trying to answer those questions.

An example for changes in questions addressed is the manufacturing industry. Like described in the proposal for the project Balanced Manufacturing (BaMa). Traditionally, the manufacturing industry focuses on availability, adaptability and productivity of production systems. However resource efficiency is significantly gaining importance. Currently, most European states are rethinking their energy policy. In the long term Europe will substitute fossil and nuclear energy through renewable energy sources. This transition towards renewable energy is a long-term project, but must be implemented as quickly as possible. In addition, energy demand is increasing constantly for our consumer society. Therefore it will come to a shortage of resources in the short term and holistic approaches must be developed to increase the energy efficiency in different fields of our society.

One of the largest energy consumers is the manufacturing industry. Therefore, the development of a holistic solution strategy for an energy saving, but still competitive European industry, is an urgent challenge due to the energy efficiency targets of the EU. In 2009 the industry consumes approximately 24% of the whole consumed energy. Just traffic with 33% and private households with 27% consume more than the industry. (http://epp.eurostat.ec.europa.eu). The members of the European Union agreed on the 20–20–20 targets (http://ec.europa.eu) which are:

- A 20% reduction in EU greenhouse gas emissions from 1990 levels
- Raising the share of EU energy consumption produced from renewable resources to 20%;
- A 20% improvement in the EU's energy efficiency.

In Austria an energy efficiency law came into force. The companies get forced to investigate their energy consumption and begin to use energy more efficiently. Manufacturing industry is confronted with disadvantages in terms of labour costs and rigorous environmental sanctions. Therefore, Austria’s (and other countries) companies have to take any chance to get more efficient in order to stay competitive on the global market.

The total energy consumption in Austria in the year 2009 was 1.057 PJ out of which 305PJ were used for heating and air conditioning and 308 PJ (29%) were consumed by the manufacturing (Statistics Austria). Especially alarming is Austria’s failure to achieve Kyoto aims for $CO2$ emissions. (Umweltbundesamt, 2011; cf. Figure 1.2)

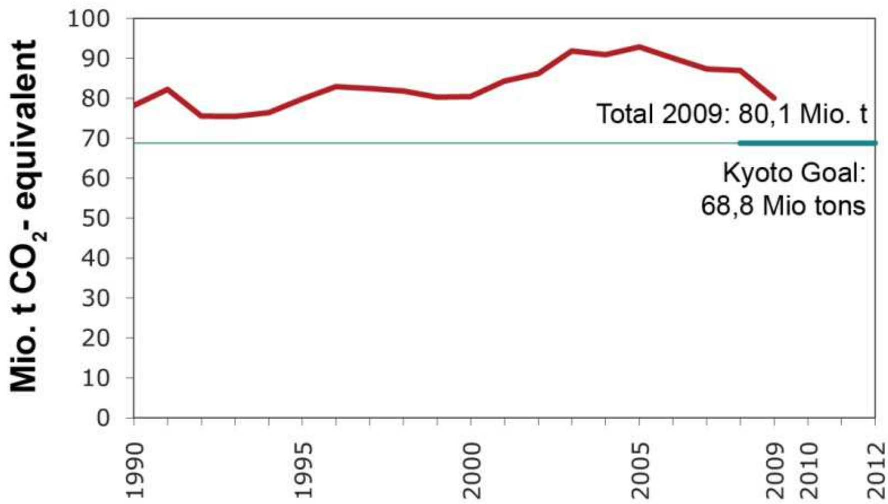


Figure 1.2: Austrian greenhouse gas emissions compared to Kyoto aims (Umweltbundesamt, 2009)

In manufacturing industries like pulp and paper, food and beverages systems of different vendors are usually used for controlling the

- production process (by PLC and SCADA systems)
- logistics and planning (by ERP and MES systems)
- building automation (by Building Automation System)
- energy consumption (by using Energy Management System)

All systems work independently and do not exchange data at all respectively just exchange a small set of data only for reporting purposes (e.g. in data warehouse and reporting tools). Due to this an overall evaluation of the complete process with all its connections between raw and auxiliary material consumption, energy consumption, production costs and product quality is not considered adequately.

Production planning by ERP or MES systems is normally done by scheduling raw material, resources and equipment considering requested end time and product quantity. Energy data for a specific product or production unit are not used in the scheduling algorithm.

So what is needed is a model approach, where a „general" energy and even better a CO2 Footprint of the whole system can be measured and combined with a simulation approach.. At the moment we have only models for subsystems of the factories: discrete models for entities running through production, models for the building itself (heating, climate), static models for economic planning.

1.1.2 Complex Decision Processes in Health Systems

Health technology is one of the fastest growing industries and is directly relevant to all levels of the population. The Austrian health care system incurs costs of over EUR 30 billion per year (Statistik Austria 2013). The bulk of the costs (77 %) are publicly financed. While the volume of health services required is increasing (e.g., because of demographic change), resources remain limited. Basing health policy and planning decisions on research evidence can help to tackle this problem. There is an urgent need for the evaluation of new health technologies, services, infrastructure, and organizational changes as well as for the development of improved technologies for the analysis, planning and control of health systems. The UK, for example, spent about 1.5 % of the health system costs on research and development in 2011 (HM Treasury 2013). A solution to these challenges, which countries face world-wide, would thus carry a market potential of up to EUR 350 million per year for Austria.

Strategy decisions influence healthcare policy for decades to come, as resources are often interlinked and all decisions will have long-term effects. Today, decision support in health care is usually based on evidence from studies of limited size, but not yet on the analysis of large volumes of routinely collected health care data ("real world" data). The reason for this deficiency is that the need for technical solutions grows with the volume of data and the number of different data sources that must be linked. Despite great advances made during the last decade, decision support technology for health policy and planning, with general applicability and reproducible solutions, is still not available.

In the last decades, methods and technologies for decision support were developed and integrated into health systems research. Still, the demand for stable analysis and prediction in order to assure high quality decision support continues to rise, just as the amount of data coming from health systems does.

Using modelling and simulation as a tool for decision making support is best practice for the computation of various scenarios with a particular focus on dynamic processes, such as disease transmission (Zauner et al, 2010a; Zauner et al, 2010b). These considerations provoked a desire to integrate more sophisticated methods of modelling and simulation into Health System Research and Health Technology Assessment.

Therefore, a need for new methods, models, and technologies subsides. These should

- be able to handle complex data sets in different aggregation levels and quality,
- meet challenges of further data processing,
- integrate different knowledge and instruments into efficient decisions,
- be highly adaptable and flexible, and
- supporting answering different questions of different stakeholders.

1.2 Motivation from System Theory

As mentioned above there is no general theory on modelling and simulation. As described in Chapter 1.1 we can assume that this is on one hand historical, as different domains have developed different modelling and simulation techniques, but on the other hand it is a “system immanent” effect. However we can just ”regognize” the status quo. In history there were some attempts to introduce a simulation theory based on system theory approaches (von Bertalanffy, 1950) or cybernetics (Wiener, 1965). But all approaches were not successful as modelling and simulation is useless “without driving applications” (Felix Breitenecker, Lecture helt 2004). Simulation is intended to solve problems and not generating a theory “searching for problems afterwards”. Problems derive from real world and we have to develop the foundations to tackle these problems on a clear mathematical and algorithmic basis.

Based on the “White Box” and “Black Box” approach described above, the question is wether we can user different approaches developed in different domains or not. So following Definition 1.2 and Definition 1.3 if we have two Mappings of models f and g in two different domains, can we compare these mappings (and resulting models) and can we exchange e.g. these methods between domains. In addition – if we follow Luhmanns approach – the problem is that these approaches are not only different in their representation, but also in their foundations, i.e. the system and the resulting problem formulation itself.

As a conclusion we have to tackle a variety of questions in the following, as different approaches have the problem that they cannot be compared. In our case we need to have y look on various aspects. There are some things to mention:

- How are Systems described and how problems are derived, according to a given domain?
- Can model approaches be compared? And if yes, what assumptions have to be made? If there is a general approach, how can we make a first iteration to model the problem with another approach and how are they related?

- If we have invented two models for the same problem - how can we handle the transfer of parameters within such models?
- What formalisms do we have to obey for future comparison of models? Is there a need and a potential for validation of the models against each other?

Today there are some dangers in the simulation communities

a) Today „Big Data“ is a „buzz word“. Solving real life problems is described as the „4th Paradigm“ (Hey, 2009). The intention is, that after „experiment“, „theory“ and „simulation“ analytic and prognostic problems can be solved by evaluating huge amounts of data. Beside a very vivid development in this area there is still believe, that the data itself would answer all our questions. The concept that the 3rd and the 4th paradigm have to be joined is already at the beginning.
b) In some cases authors present their approach as the ultimate solution (Wolfram, 2002) but as a matter of fact it might well be possible, that a lot of systems and problems can be tackled with one or the other model concept. Nevertheless this is no proove, that this attempt is „the optimal concept“. We can se very often that approaches are only different in their formal representation, but are equal in concept and final implementation. Especially Cellular automatons are only one possible representation of a formal model concept, which goes much further.
c) Using concepts from „White Box“-Modelling and „Black Box“-Modelling, there is always the temptation of reducing formal and mathematical needs for models for various „domains“. Very often model concepts are formalised not very well, and instead of introducing hard approaches from technical point of view, weaker concepts are introduced the other way around.
d) Described approaches of „integrated“ development, need even more communication than before. As a matter of fact the formalisation of transfer between domain immanent modelling concepts is not leading to fully automized concepts, but generates the need of interdisciplinary communication. And as we learned from Luhmann, it is not sufficient just to translate models already developed, but we have to go one step back and define the generated system/problem new to develop a „joint model approach“.
e) Despite all approaches of a general model theory we can only collect mosaic stones, always missing the most important parts.

Intuitive one could say that modelling and simulation is a tool for solving problems and answering questions that are related to a certain system, in our words a domain. The method consists of creating a representing model, formalising and simplifying it, implement it and performing experiments, so called simulations. Simulations, in this sense, shows the behaviour of the system under different circumstances, which may be formalized as input and initial state.

Starting from Systems, they are defined in literature in a wide range. Informal definitions have the advantage that they are useful to describe a lot of possible objects. When it comes to the general concept of a system definitions include mathematical, mental and physical systems. After Definition 1.1 we take a closer look on other approaches:

Peter Fritzson defines *„A system is an object or collection of objects whose properties we want to study."* (Fritzson, 2004) and von Bertalanffy defines a system as *"a complex of interacting elements"*. (von Bertalanffy, 1950) Interaction means that there exists a relation R between the elements and that it influences their behaviour (i.e., the elements would behave differently if they were in no relation or in a different one). The system is therefore more as the sum of its parts, and moreover, understanding the behaviour of each element in isolation is insufficient for deducing the behaviour of the system as a whole. In this definition of system we can already see the first traces of the definition of complexity, as it was developed in the eighties in complexity sciences. Bernhard P. Zeigler makes in "Theory of Modeling and Simulation" the simple assumption: *„A system is a potential source of data"* (Zeigler et al, 2000).

These formulations are probably some of the most simple definitions in literature, but the already indicate a difference in the point of view of the first step in the modelling process: "To define how reality is seen as a system" One can have the point of view, that systems are objects, on can see the relations (both views representing the concept of a "theory" behind it), but one can also just see "data", which more or less represents a wide represented view today.

To go a little more in detail there are differences in the understanding of systems, e.g. a dynamical system. Different authors use dynamical system for all systems that have time-dependent behaviour. Sometimes in literature a state space is required. Very often only input-output systems are considered, while this of course is a shortening of the meaning of the word system.

Zeigler cited above with the data point of view of courser invented one of the most important methodological concepts for hybrid modelling since the 70ies until today. He defines a system in the form of *source system* and view it as "the real or virtual environment that we are interested in modeling". A simulation model "is a *set of instructions, rules, equations, or constraints for generating I/O behavior*" , where I/O is input output behaviour. The Austrian author Franz Pichler proposes another perspective for models as scientific descriptions of real phenomena, and here systems are always formal scientific constructions that either serve to simulate the behaviour of the model or are proposed as a basis for model construction. (Pichler, 1975) These two tasks are the endeavour of systems theory and so systems can serve as representations of models and not the other way around. They are always formal constructions and Pichler does not speak of the real phenomenon as a system. In our terminology, the equivalents to these formal constructions are the mathematical systems. The assumptions and definitions on general system were developed with the research group. It is the basic idea to improve the common basis on these concepts within our group. Patrick Einzinger, who focussed in his PhD thesis on the comparison of Agent Based models and System Dynamic Models as an example for comparative Modelling, summarized the Definitions already (Einzinger, 2014)

Mathematical systems are studied because they can be used as models for real systems, but we want to treat certain objects of the physical world as systems, for example a industrial production plant, the population of a country, or its health care system, but physical objects are not mathematical objects and cannot satisfy a formal mathematical definition. Therefore we are looking for a definition of systems, and then a formal definition of the special class of a mathematical system. What constitutes a model will also only be formal if all involved systems are mathematical systems.

Definition 1.4 (System II)**.** A collection of interacting or interdependent objects is called a system. The objects are the components of the system.

Most systems interact with the outside world rather than exist in isolation. Their system boundaries separate them from the environment. A system can still interact with its surroundings by the input that it receives and the output that it generates. We call such a system an open system, opposed to a closed system, which exists in isolation (von Bertalanffy, 1950).

There are two important aspects of a system: its structure and its behaviour. The structure describes the components and how they are interconnected. What follows from this structure, the outcomes that the system generates under various circumstances, constitute its behaviour, which can be measured in the form of data. (Zeigler et al, 2000,) emphasize this role of a system as "a source of observable data".

The system that is the actual object of interest (source system) will be denoted by Σ_O . Structure and behaviour of Σ_O are probably complicated, hard to understand and hard to experiment with, in particular because usually it is a system from the real world and includes physical objects. A model system Σ_M that is in a certain way similar to Σ_O , but simplified and easily accessible is preferable to work with.

Σ_M should be related to Σ_O in some way. Let us denote by C_O and C_M the sets of components of the two systems. Then (Ferstl and Sinz, 2013) require the specification of a model mapping $f\colon C_O \to C_M$. One can also demand that f is a homomorphism if both C_O and C_M have an algebraic structure, which is the algebraic modelling approach, in contrast to the general approach without the requirement of a homomorphism (Mesarovich et al, 1975).

Even without that, there is a problem with this approach of mapping the structures of two systems. Suppose the system of interest is a specific country or, more specifically, its human population. A single differential equation for the number of humans in the country might be our model system. The components of this model system might be the number of humans (a state variable), the change of humans per time unit, the number of births per year as a constant, and possibly others. What would be a good model mapping? Every human can be seen as a component of the object system, so f has to map him or her to a component of Σ_M , and naturally this will be the number of humans. However, there might be components for which we do not want to have a counterpart in the model system (e.g., the animals, trees, and buildings of the country). No component of it is a reasonable image for an animal. In the model, they are unnecessary. A better approach is to map behaviour instead of structure. Suppose we observe a particular behaviour b of Σ_O , then for Σ_M there should be a counterpart b^l. In the example above, b might describe the development of the country over time, including its population, animals, trees, buildings, and all other components. The corresponding b^l of the model system only describes the number of humans at every modelled time point. Two different possible behaviours b_1 and b_2 of Σ_O will be mapped to the same b^l as long as they give always the same number of humans. The mapping ignores the behaviour relating to components that are of no interest. In the following definition, we assume that every system has a set of all its possible behaviours, the universal set of behaviour U.

Definition 1.5 (Model II). A triple (Σ_O, Σ_M, f), where Σ_O and Σ_M are systems and $f : U_O \to U_M$ is a surjective mapping, is a model. We call Σ_O the object system, Σ_M the model system, and f the model mapping.

A model consists of three parts, two systems and the model mapping, but less strictly one can also speak of a system Σ_M as the model of the system Σ_O . The model mapping is then only implicit. This is the usual way in which the term model is used, in particular because a model mapping can only be formally defined for formal systems. The focus on behaviour instead of structure is influenced by the behavioural approach to systems theory (Willems, 1991).

In Balci´s "Validation, verification, and testing techniques throughout the life cycle of a simulation study" (Balci, 1994) the relation between "system" and "model" is also described. Balci mentions model and system Input Variables and model and system Output Variables. In addition there are model and system Parameters.

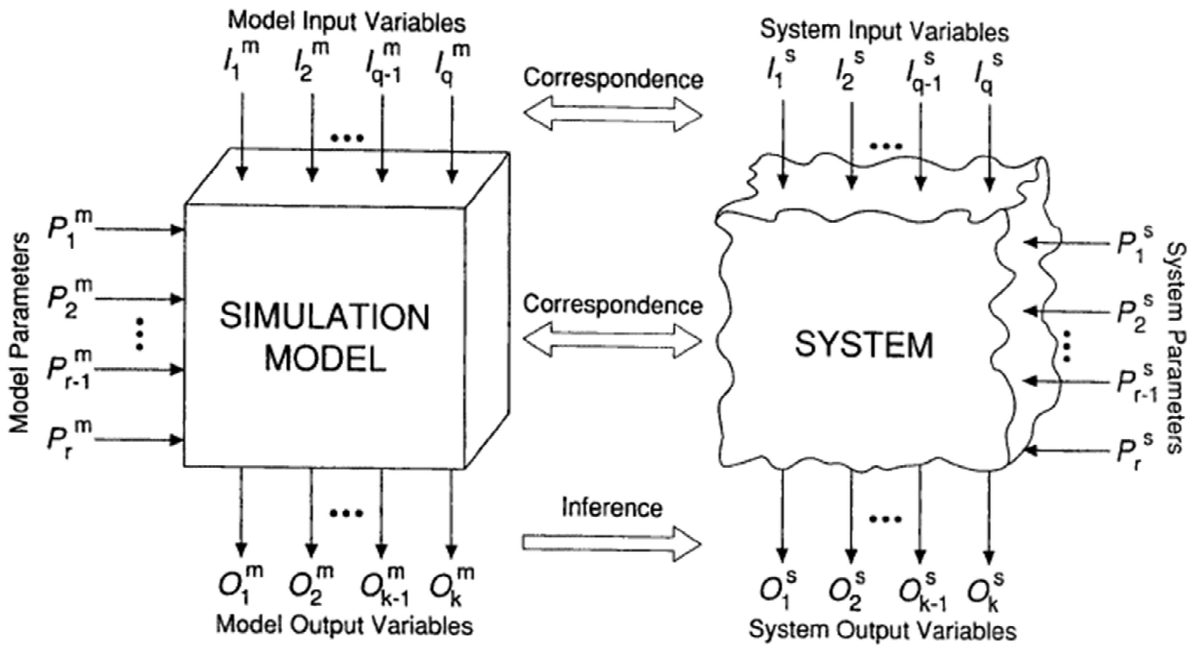


Figure 1.3: Concept of I/ Systems and I/O Models by Balci (Figure originally from Balci)

For getting a model there is bottom-up development, where model construction starts with the sub models at the base level (i.e., the ones that are not decomposed further) and culminates with the sub models at the highest level." and "In top-down development, model construction starts with the sub models at the highest level and culminates with the sub models at the base level (i.e., the ones that are not decomposed further)."

Based on the made assumptions and definitions we will define the concept of a „Problem" instead of System because of domain related, practical modelling tasks, we normally define our task in three well defined steps.

As a first step we analyse given data within a system. Regarding tot he domain, quality and quantity of data will differ. Data is needed not only, for parametrisation but also for validation and verification and many more aspects. Later we will describe the concept of standardized processes in simulation tasks for generating parameters out of given domain data. As a second step we analyse the system knowledge, so we assess all given structural and behavioural information of a system. This information might be homogenous or heterogenic and will result in one model or in a model (or simulation) which will be divided into sub models or sub simulations. Last but not least and as a third step we have to discuss the research question for our model and the resulting simulation. As an example in Health Technology Assessment and Evidence Based Medicine such research questions have to be defined as PICO questions (Gerber 2006).

Definition 1.6 (Problem)**.** A well-defined research question, based on analysis of given domain data and system knowledge is called a problem. The problem can be analysed with one or more models.

1.3 **Summary of Goals**

In the following chapters we will, based on the abover described motivation and ideas, describe the recent approaches for improving the capabilities to compare models. We will focus on aspects of developing modelling techniques for improving these abilities on the one hand. On the other hand examples will be taken mainly from the two domains "Complex Functional Infrastructure" and "Complex Decision Making in Health Systems". For this reason I will summarize no the goals in this areas.

1.3.1 Goals for Complex Functional Infrastructure

In Chapter 1.1.1 some motivations from the domain of complex system in functional Infrastructure were described. As an example we take the funded project BaMa (Balanced Manufacturing), initiated by the Institute for Production Engineering and Laser Technology 2014. Based on the motivation described the goal of Balanced Manufacturing is to develop a method and it's technical implementation in order to monitor, predict and systematically and interdisciplinary optimize the energy demand of manufacturing companies under comprehension of the economic success factors time, cost, quality, hence it is called "Balanced". BaMa will support energy efficiency in two ways: directly via the optimized plant operation and indirectly via identification of the largest optimization potentials. The implementation and evaluation takes place at selected industrial partners of in the industrial surrounding of the metal processing and food sectors, so the practicability of the concept is proven.

First step of the project was to develop the Balanced Manufacturing Methodology. The methodology can be seen as a guideline for preparatory system analysis. Hereby a modular approach is chosen: the production facility is seen as set of various basic modules - cubes, for each of which boundaries towards the surrounding and other cubes is defined. This approach offers various advantages:

- Generic description of cube attributes offer versatile applicability of the method to different industries
- Exact placement of sensors and measuring equipment and energy-flow capture at cube interfaces
- Data obtained from the cubes is of fine granularity and can be aggregated in different ways to extract useful indicators
- Modular system architecture offers flexibility and reusability of software parts

In addition to the cubes a significant product-footprint will be described. The product-footprint is the core reporting tool within Balanced Manufacturing. It represents the products expenditures concerning the resources cost, time, energy and the environmental impact such as resulting carbon emissions in the product life cycle phase within the factory and relates them to the product-related success factors (as quality, price, credibility) in order to achieve a sustainable and competitive production. Every cube that is involved into this process adds to this product footprint. Relating the resource consumption to the product offers two main advantages:

- Knowledge of energy demand of the production steps in relation with a production schedule makes the energy demand predictable
- The product-footprint can further be directly used as novel sustainability label.
- Especially since it can be anticipated that the legislative authority will demand some kind of energy certificate for products within a conceivable horizon of time the product-footprint provides valuable preliminary work to enable companies to deal with this challenge.

The Balanced Manufacturing Methodology and the product-footprint systematic will be documented in s set of guidelines and published.

Based on the modelling and simulation point of view, by doing so we have already defined some important aspects. Based on the given domain, we have defined clear defined research questions. The need for new approaches in modelling results from the extension of the system and the new definition of research questions. Last but not least in this case the simulation will be needed to interact with "hardware in the loop" i.e. the monitoring systems of the production plants. The planned methodology already will fulfil our need for a "mathematical system" or at least a formal system.

The second main objective of the project is the development of a tool-chain for energy efficient operation and design production plants under competitive conditions with minimal energy and resource consumption – Balanced Manufacturing Control (BaMaC) tool. The BaMaC will be developed based on the BaMa methodology and upon the insights gained through analysis, measurement and simulation. The Balanced Manufacturing Control will consist of three core modules:

Monitoring: the data about resource consumption acquired within the cubes will be aggregated and visualized in an appropriate way to support decision making in energy related terms. This part of BaMa fulfils the compliance of energy monitoring specified in ISO 50001 in a way that is compatible with the rest of the system and completes the BaMa tool set.

Prediction: this BaMa module predicts the overall energy demand of the plant based on the product-footprint and a production schedule.

Optimization: Based on data models and numerical simulation models of the cubes this part of the tool chain will be optimize the plant operation with regard to the optimization targets provided by the management via a target product-footprint. It will support energy efficient decision making in two ways: directly by suggesting an optimized plant operation strategy to the user and indirectly by identification of the largest optimization potentials.

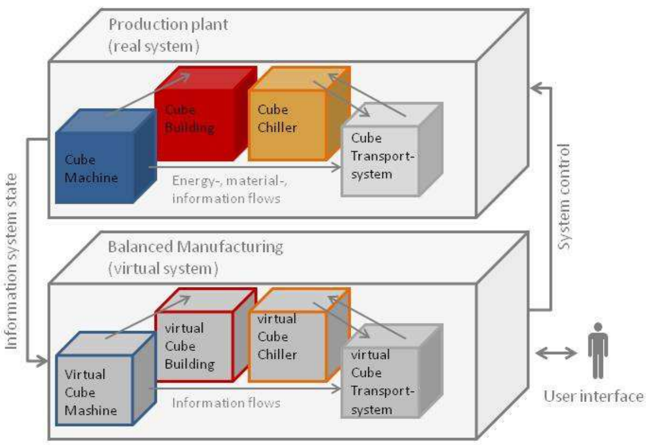


Figure 1.4: The BaMa Concept with „Cubes" as defined in the proposal oft he BaMa Consortium lead by the Institute for Production Engineering and Laser Technology, TU Wien

For data acquisition, a **measuring and experimental cube**, as representative production-unit or manufacturing cell is used for detailed measurements and analysis of energy- and resources flows. Furthermore an extensive rule base containing models, target functions, formulations for constraints and optimization strategies should be formulated. This rule base should be platform independent.

Based on this rule base software to realize Balanced Manufacturing Control should be developed in connection to existing automation and software systems. So in summary - from the modelling point of view - the task is to develop a method for modelling the described processes based on complex system information, complex data collected by the "real life" cube. For doing so the method should be able to transform the real life into a system (defined by so called cubes) and then transform these cubes into a computable model.

A lot of boundary conditions have to be obeyed. In the first phase the specific requirements for the Balanced Manufacturing are defined and based on them a methodology for the system analysis of a plant in the sense of BaMa are developed. Use case definitions for the specific needs of the potential Balanced Manufacturing users are defined in close collaboration between the scientific and industrial partners. Therefore an investigation of the industrial partners target areas, goals, plants, boundary conditions were conducted and literature, related work and projects have to be assessed for valuable input.

Based on the previous findings a methodology for conducting a system analysis of a production plant in preparation for the implementation of Balanced Manufacturing is developed. It is aspired to formulate this methodology at a generic level to ensure its usability in a variety of production facilities. A basic element of this system analysis consists of the cubes. Cubes constitute subparts of a system with defined boundaries, interfaces to other cubes, a certain physical behaviour that contributes to the energy balance of the system and usually some degree of freedom to be influenced for optimization. In other words the boundaries of sub systems in terms of energy-, material- and information flows are defined to intersect the whole system into observable parts. The characteristics and attributes of cubes are defined in a generic way in order to guarantee the applicability for all parts of the plant and for different kinds of productions. A cube can be for instance a machine tool, a chiller, the building or a baking oven.

Parallel to the definition of the cubes a product-footprint is defined, which sets the product success factors in context with its ecological footprint. In particular the resources energy, costs and time will be captured and visualized for the transformation process a product undergoes within the plant. Each cube that contributes to the product's energy, cost or time consumption within the production plant, which accumulates to the product footprint. Therefore, the product-footprint is made up of a high number of originally independent data streams that aggregated in a time-synchronized manner. Methods for suitable data aggregation and fragmentation will be found and described.

One problem to be handled is that as BaMa should be a general system, with complex data to be integrated, the model process has to be extremely stable. Data from various sub domains has to be integrated. Measurements that cannot be performed at the experimental cube will be taken at the industry partner plants in order to complete the measured data basis. Energy flows which cannot be measured at either the cube or the partners' production plants will be simulated, e.g. with physical modelling the integrated simulation which was already developed. So the basic idea is not to implement directly a model, but to see the cubes as a mathematical system and "parent model" for structured models which can be implemented later on. The ideas for this concept will be described later in the area also for a completely different domain, for infectious diseases.

1.3.2 Goals for Complex Decision Making in Health Care

As described above health is our most important value. Therefore, decision-making for health care is a crucial task, which still grows in importance. To tackle this goal would be to help all stakeholders reach clear, transparent, and efficient decisions with new methods, models, and technologies. So a process is needed, which supports the incorporation of clear and predictable requirements for providers and payers in order to deliver the best possible and affordable services to all patients in an affordable health system. So the development of decision support methods, models and technologies is needed, that are based on data collections in health systems. However, the solutions found should also be applicable to other areas.

One characteristic of the approach should be that the focus lies not only on single specific questions or stakeholder views, but also on a more comprehensive viewpoint. The concept should develop methods, models, and technologies for a range of questions and will thus enable a variety of stakeholders to implement new collective decision making processes. For this it is aimed to develop methods, models, and technologies, which

- increase the possibilities for measuring, planning and controlling a health system,
- raise the quality of decision-making for health systems,
- ensure the privacy of patient data, and

- guarantee the transferability of methods, models, and technologies.

It should provide them to various stakeholders, ranging from scientific partners of all areas to economic partners, such as providers and national and international decision-makers.

Based on existing routine data, the task is to integrate all relevant domain knowledge in order to address this challenge and develop methods for data handling, modelling, and decision support. It focuses on a clear research field that remains accessible to complementary development and the integration of additional cues. This would open up future research potential in promising fields such as the integration of broader data sources or dynamic modelling.

From the modelling point of view, so the whole simulation process starting from given domain knowledge and complex data sources over model selection and coupling up to the visualisation and assessment of resulting simulations has to be obeyed. So the idea is to structure the overall concept into three "topics", which are devoted to the technological processes that are necessary for decision support.

- **Topic "Data"** Research and development of data provision methods and services
- **Topic "Models"** Research and development of innovative decision support models
- **Topic "Decision Support**" Integration of tools for decision support, scientific and industrial transferability, and quality assessment

In the last decades, methods and technologies for decision support were developed and integrated into health systems research. Still, the demand for stable analysis and prediction in order to assure high quality decision support continues to rise, just as the amount of data coming from health systems does. Therefore, a need for *new methods, models, and technologies* subsides. Methods should

- be able to handle complex data sets in different aggregation levels and quality,
- meet challenges of further data processing,
- integrate different knowledge and instruments into efficient decision processes,
- be highly adaptable and flexible, and
- support answering of different questions for different stakeholders.

The resulting process should be structured in three areas to clearly address the challenge of developing new approaches for tackling the pushing questions. The three topics "Data", "Models", and "Decision Support" represent the main steps in the process of supporting decisions in the health care system, where specific knowledge and experience from different partners has to be included. Various new approaches will be designed and tested, so the framework must be ready for integrating all these approaches. A main idea is to combine and link those efforts for the development of fundamental new strategic results.

The topic "Data" should focus on the challenges of working with complex, large and sensitive data sources. Therefore, it should provide new technologies for the task "Data Handling" such as preservation, standardisation and enhancement of information. "Record Linkage" should be another task in this topic, as health systems research faces enormous challenges of fragmented data sets not only (but especially) in Austria. The third important task is "Data Quality", where new strategies for profiling, assessment, documentation and monitoring should be developed. This should also enhance the quality of the other topics, which are based on data. The fourth task is to ensure "Privacy" of patients' data via pseudonymity, (k-) anonymity, and legal issues.

The topic "Models" should oversee a wide range of possible analytic methods, including not only dynamic models, as described above, but also new statistical and analytic methods for the task "System Analysis". These findings have to be joined with distinguished experience of health systems research to develop a variety of system knowledge focussing on the aggregation of information as well as static („status quo") and dynamic (history and future scenarios) analysis. Based on the analysis and knowledge of the system, new models for analysis and prognosis to support the decision process have to be developed and methods for validation & and assessment of the quality of results for the practical and methodological assessment of the developed methods and technologies has to be developed. An additional demand is the reproducibility of complex models and simulations, which should have a major influence on the sustainability of developed methods, models, and technologies. This task should also include the question of dissemination of sensitive results to the scientific community.

The topic "Decision Support" should be a derivative section of the used models and should integrate all aspects described above to develop application oriented solutions. Delivering the new developed technologies to the decision makers via well-defined methods & tools should challenge the developers in converting developed models into reproducible quality proved simulation tools.. Stakeholder-oriented representation of results, visualization of complex scenarios and development of methods for feedback processes to integrate new insights into the process of decision making in the health care system have to be addressed.

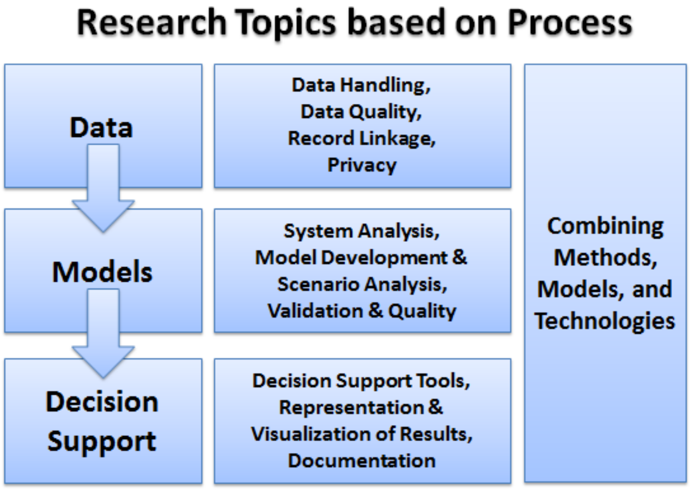
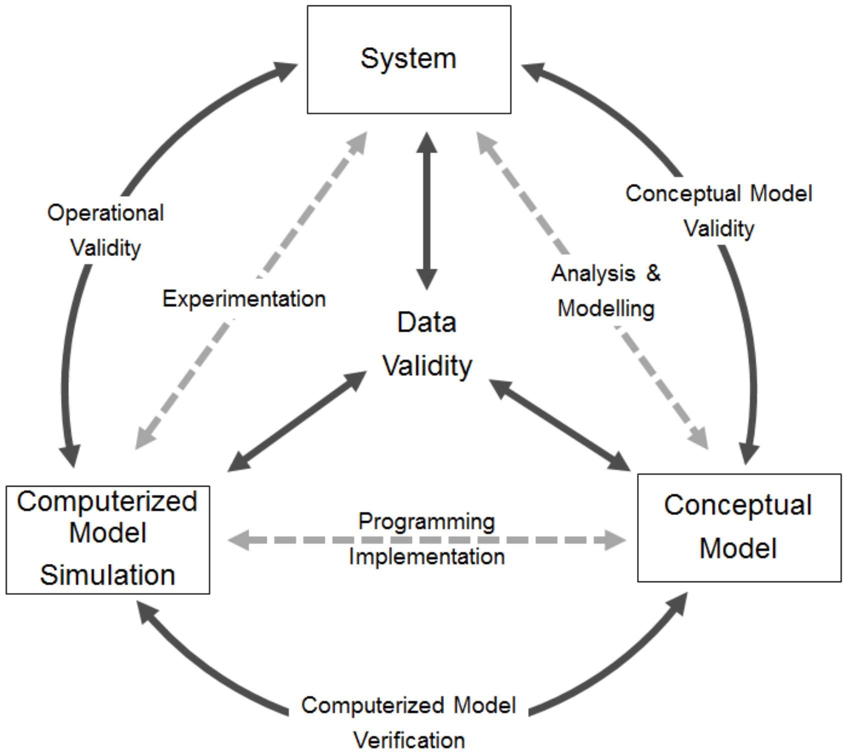


Figure 1.5: Planned Structure of the Simulation Process

With basic approaches these planned structure was to possible to be implemented. So - for dealing with the described goals - our research group developed two research projects. IFEDH (Innovative Framework for Evidence-based Decision support in Healthcare), which should be described in Chapter 4.1, introduced the basic concept for development of an integrated simulation pipeline, based on the modelling and simulation concepts. In addition the now running project DEXHELP, which was introduced by the author in 2014 combines the described concepts in a long standing system, which runs the defined concepts in a big scale.

2 The Modelling Circle

Based on the characteristics and demands described in Chapter 1, Chapter 2 contains some aspects of the classical modelling circle and its limitations regarding to our needs. If we have a look on the classical modelling Circle we can take e.g. the one which was presented by Sargent (Sargent, 2012)



It presents the more or less classical approach, where we start with the „real system“. By analysing this problem we get to the next step modelling the problem to get a „Conceptual Model“. After this we get then by programming and implementing the model a „Computerized Model“ or a Simulation.

This concept fulfilled all need aspects for a lot of years, but for today’s needs some important aspects are missing.

2.1 Cellular Automatons and Diffusion Based Equations

As a first example a short outline of a modelling approach shall illustrate some of the concepts I will try to address in this work. The article "Diffusion-based method for producing density equalizing maps" (Gastner & Newman, 2004) presents a model description of a diffusion based model in the more or less “abstract” application area dynamic cartography. The basic idea was to analyse this model approach (this work was done together with my colleagues M. Bicher, S. Winkler and I. Hafner) and to develop another model, so that it uses directly a cellular automaton (CAs) that simplifies the formal description and can easily be implemented.

This approach should illustrate the question whether this approach is a different implementation of the same model, a different but similar model or if it is a simplification of the model taken from literature. For the first part of the question: In our case we explicitly do not want to use CAs as numerical solution of the given model, but want to introduce a stand-alone modelling approach, which should be compared to the original one. We chose the application of cartography, as there is no „real world system“ for the question of density equalizing maps to be compared, so we could let this aspect out of focus for the moment (see "Modelling Process" later) and we can focus on the comparison of two models.

Diffusion Based Method

First I want to describe the intention of the diffusion based method for the density equalizing map. In the article of Gastner and Newman the idea is to create a map that does not reflect the size of the countries as it is, but should visualise other parameters, such as the number of cancer diseases (cancer prevalence) via the size of parts of a map. Of course the first idea would be to visualize cancer based on points. It would look like this:

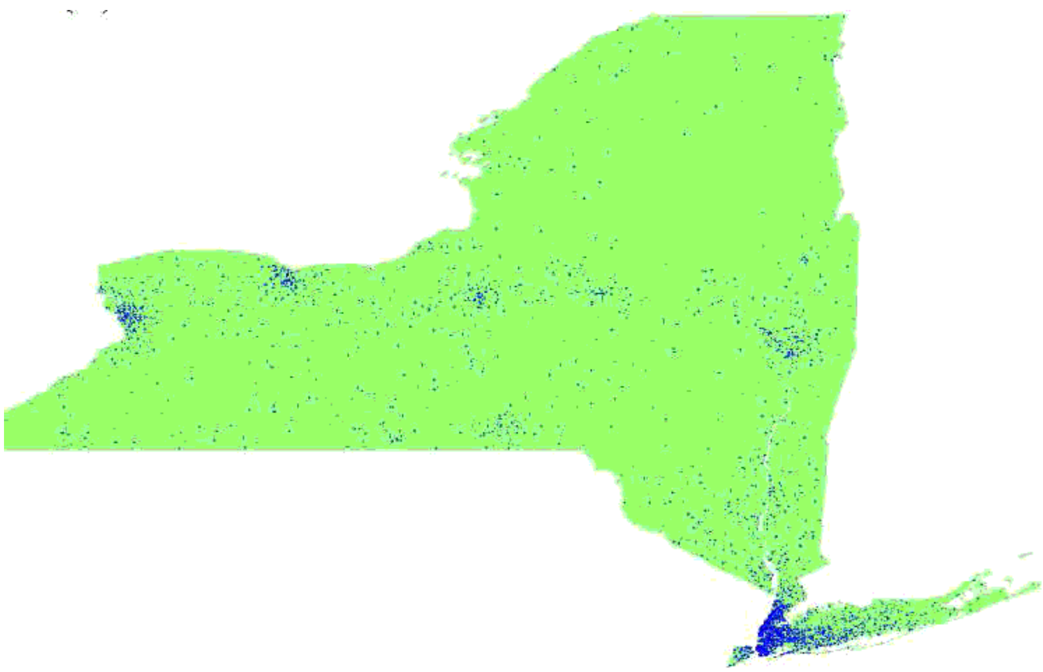


Figure 2.1: Lung cancer cases among males in the state of New York 1993-1997.

In Figure 2.1. aach dot represents ten cases, randomly placed within the zip-code area of occurrence. (Original Version by Gastner, M. T., & Newman, M. E. J. (2004). Diffusion-based method for producing density-equalizing maps. Proceedings of the National Academy of Sciences, 101(20), 7499–7504) At first glance, one would think that in New York City there are more cancer patients than in the rest of New York. In principle of course this is true, but we cannot say that cancer in New York City is more likely than in rural areas, because there live a lot more people than elsewhere on this map (of course New York is a very good example for different population densities).

The purpose of Gastner and Newmans model is to identify places where certain matters are more likely and to make the geographical allocation and number of cases per head visible, i.e. to construct a map where subsamples of the population are visualised proportional to the population in this area. In areas with the same per capita incidence there should be the same density. So the map should be scaled according to the subsample of the population (or other characteristics) in this area. This principle is called cartogram.

The population (or another) density function can be defined in several ways: One way is to divide the area considered in policy areas, and the people living there are spread evenly over the areas. The smaller we assume these regions, the more accurate is the resulting map. As we can imagine one interesting aspect of these cartograms is that the original form of the countries is lost, as you can see in this example taken from the original article.

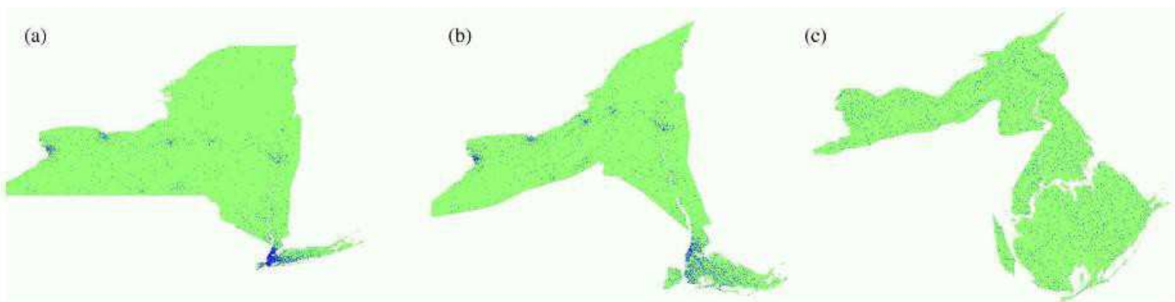


Figure 2.2: Different Cartograms of coarse-grained population density

The maps describe as above the lung cancer prevalence of the male population in New York from 1993 to 1997. The left part of Figure 2.2 shows the original version, (b) a cartogram using a coarse-grained population density with σ= 0.3° and (c) A cartogram using a much finer-grained population density. (Data was taken from New York State Department of Health - Original Version by Gastner, M. T., & Newman.) The left part of the figure shows the original proportion of New York. After uniform distribution of cancer cases and scaling of the map, the dots are distributed uniformly, but the outlines of the map are no longer recognizable. This visual concept is even more interesting, when we look on a country, its outlines and the change of its federal states.

With the aid of physical diffusion equations, a model of this type was created by Gastner and Newman. This model is elegant, intuitive, well-defined and at the same time it requires less computer resources as experimental models using other existing methods (see Gastner & Newman, 2004). A map whose countries should be proportional e.g. to the population, demands by definition that the population density must be the same everywhere.

To create this map, you have to allow the population to "flow away". This model is based on the "Fickian diffusion". The diffusion is achieved with the flow of population from areas with a high density in areas with a low density via density compensation. The population is described by the probability density function $\rho(r,t)$, where r is the geographic location and t indicates the time. At time $t = 0$ the density is unequal distributed, big cities like Vienna have a higher density like rural areas. With the progress of time, the diffusion process starts, where direction and amount that may flow, is given by $J = v(r,t)\rho(r,t)$. The flow is determined by the gradient $J = -\nabla\rho$. Is the rise steeply, the population flows faster. Local behavior of the diffusing population is $\nabla J + \frac{\partial\rho}{\partial t} = 0$. Combining these three formulas, we arrive at the well-known diffusion equation

$$\nabla^2\rho - \frac{\partial\rho}{\partial t} = 0 \qquad 1.1$$

with the velocity cell

$$v(r,t) = -\frac{\partial\rho}{\rho}, (1.2) \qquad 1.2$$

The total displacement of a point is described by the equation

$$r(t) = r(0) + \int_0^t v(r,t')dt'. \qquad 1.3$$

Finally we have to think about boundary conditions at the borders of the countries as well as the, usually rectangular assumed, borders of the whole simulation area.

Regarding the first issue, we need to watch the area around the considered countries. Let us consider a virtual sea around our country. In reality the sea of course has no human population. But if the model is computed with density 0 for the sea, the countries would diffuse into the sea, because the flow of high density is to low density. To avoid this all unpopulated areas, such as water or the environment of the observed area, they will be assumed to have the mean density which conserves their area for the complete simulation progress. This avoids that the country is limitless spread on the water. The imaginary sea should have a multiple size of the analysed countries in order to ensure an undisturbed diffusion. Regards the latter issue we need to apply homogeneous Neumann boundaries at the edge of the total simulation area to conserve the total volume of the content. In case a map of the whole world is simulated, one can also use periodic boundary conditions.

Cellular Automaton Approach

In our alternative approach our countries are mapped to a discrete grid and the changes effected will be driven by discrete rules. A cellular automaton consists of a discrete lattice of identical cells; each is in one of a finite number of states. The dimension of the grid is finite. Time is also discrete, and the state of a cell at time t is depending on the states of a finite number of cells (the neighbourhood of the cell) at time t − 1. The neighbourhood is classed as either Moore or Von Neumann neighbourhood. The Moore neighbourhood comprises the eight cells surrounding the central cell on a two-dimensional area, during Von Neumann comprises the four cells orthogonally surrounding the cell. In the transition function it is precisely defined how the transition from one state to the next state takes place. The transitions of the states are made for all cells with the same transition function simultaneously.

Using this approach of replacing a model with another model the first question is, whether a cellular automaton can be seen as an alternative model or the implementation of the equation based concept. As a matter of fact in this chapter we "think" of it as a modelling concept – but of course this is still no proof, we will discuss this later. The second question is how limits and features of the "original model" can be shown in the implementation of the model. Parameters have to be transferred and there are certain features of the model, we want to rebuild. In chapters later on we will discuss the possibilities of comparing models and finally will define the concept of cross model validation (which is not the same as cross validation).

In the process of defining an alternative (or simplified) model, which should satisfy the features of the original model the first step necessary is to define "conditions" of our model, that have to be satisfied. (We use "simplified" at the moment not as a clear defined term – as we cannot measure simplicity at the moment in terms of which approach is more accurate). It appears that (1) the total volume ($\int_\Omega \rho(x,t)dx$) of the country under consideration must remain equal before and after application of the algorithm, as it is also modelled in the original approach. This means the conservation of the total area of the "system" analysed. As a matter of fact this appears interesting, as this feature is not always given for cellular automatons e.g. "Game of Life". Only changes allowed are shifts in the interior so for specified areas of the country e.g. federal states. However, it is also allowed and possible that the borders of the country itself change, as we also embed the system/country in a sea surface. (2) The visual appearance of the change of boarders of parts of the country should be similar in our new approach with CAs to the original model.

The first idea for the implementation of such a simplified model would of course be to use the formulas from the article. For every cell in the grid it is possible to define a point in the middle, with which we would then calculate the first derivatives in the sense of the difference. With the above-mentioned velocity cell, i.e. the first and second derivatives of the density function, calculation of the amount and direction of the diffusion would be possible.

Then the result could be assigned to the cells of the cellular automata. However, this would not be a different modelling approach, which is based on the principle of cellular automata, but would be continuously calculated values converted to a discrete problem – so we would have the classical approach of a discretization process when implementing a given model description of a system.

In opposite we want to use the modelling principle from the paper, but not yet the simplified solution. So we had to find a more natural behaviour for the cells. The stronger cells, in our case the federal states with higher density, have the power to steal parts of the counties with lower density. The exact model structure was developed and refined with the help of rules of the game "risk" and focused on implementation of the given features of the original model.

To test model approaches which fit the original model best, three different CA models were developed, where - concerning structure and principle - all three models are the same a cellular automaton. A cellular automaton consists basically of a grid, which is represented by a matrix. This approach is sufficient for the moment, we will see why this explanation is not sufficient and will define it exactly later. In each matrix entry or grid point, a state is stored. These states are influenced by the states or neighbouring cells or records. The difference of the first two models is the neighbourhood, i.e. deciding which adjacent cells have an impact on the status of the observed cell. The first model uses the Neumann-neighbourhood,

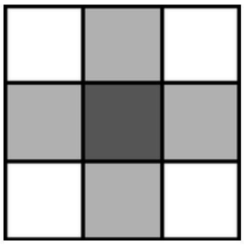


Figure 2.3: von Neumann Neighbourhood

the second approach is a Moore-neighbourhood:

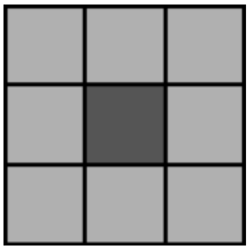


Figure 2.4: Moore Neighbourhood

The third model also uses the Neumann-neighbourhood; however, a density-dependent "switch" was be installed. Before going into more detail on this switch, which allows us to fit the given model features of the original model we consider the basic principle of the models.

Imagine a country's map embedded in an imaginary sea and put a fine grid over it. Each cell of this grid is implemented as an entry in a matrix. In our case the value of the matrix entry describes the density of the corresponding surface cell on the map. As we would cluster it for federal states, all cells within a federal state would have the same density. With this concept and considering the area of the individual federal states of Austria each entry of the matrix is 1 and the density would be all over the map the same size as the map accurately reflects the area ratios. The designed algorithm applied to the map of Austria would not change

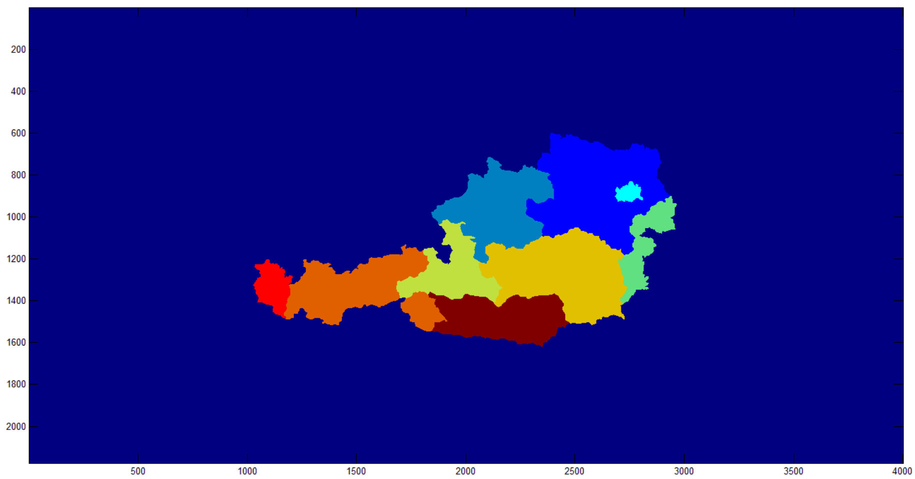


Figure 2.5: Cellular Auotmaton Approach, Basis Map of Austria

anything.

Here you can see very nice that Austria is embedded in an imaginary sea to allow the spread in all directions. Considering, however, the density would be defined by the number of inhabitants of the individual states, the matrix entries would be in the area of Vienna, much higher than the matrix entries for Burgenland, as Vienna is more densely populated than the Burgenland. The algorithm applied to this example of course affects the appearance of the map.

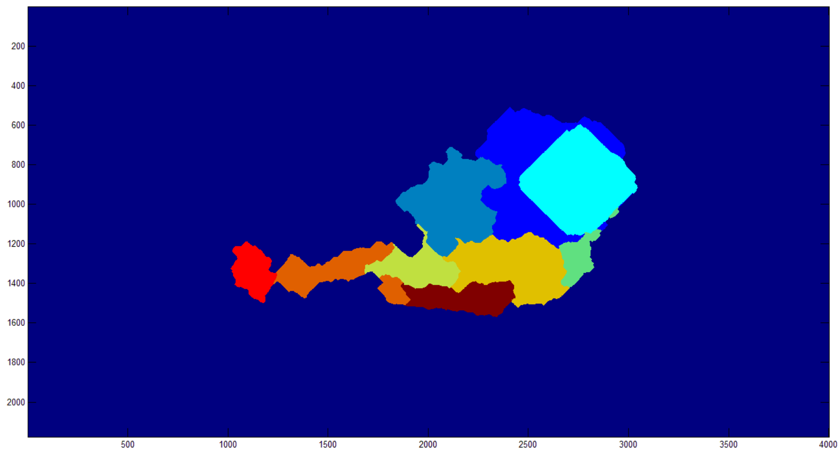


Figure 2.6: First Application with von Neumann Neighbbourhood

One can already read out from the vector that inflates Vienna enormous and because of the Neumann neighbourhood takes at magnification a diamond form.

The algorithm obtains a vector in which the values for all federal states of Austria are included considering special values for a given question. Let us consider beer consummation. For our model these values are the beer volume drunken per area. Of course values that are specified per head are no problem by computing the beer per area value with the population density values.

The CA update algorithm starts with the first array entry of the map. For each matrix entry or each cell, the algorithm considers the mentioned neighbourhood (von Neumann or Moore). If the considered matrix entry is greater than the entry of the neighbourhood, the cell with lower value will be captured by the federal state with cells with higher values.

For example, consider the above shown Neumann neighbourhood, where B denotes the cells of Vienna and A the cells of Lower Austria. Now, consider the population as a scenario, it would be clear that the entries of A-cells would be higher than those of the B-cells. If the algorithm now reaches to the marked dark cell B and checks the values of the foreign neighboured cells A, the City of Vienna would to get these two cells of Lower Austria, as the entries in these cells are be lower than in the observed B-cell. If the entries of A cells would have been higher than in the currently considered cell nothing would have changed, because only

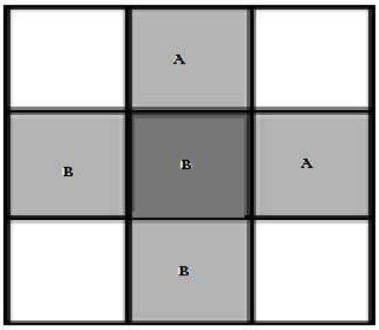


Figure 2.7: von Neumann Neighbourhood Update

cells with lower entries pass into another state. The algorithm now applies the CA rules step by step for the whole automaton or the whole matrix. Modifications are saved, using two matrices and a vector. In the vector the total number of "owned cells" of every single federal state is saved. If a cell is taken over by another federal state, it stores these changes. In one of the matrices are all density values, the other matrix contains colour codes for the federal states the cell belongs to at that moment. Of course, it happens that a cell will be overwritten during the algorithm several times, but only the result at the end of a whole array traversal will be used. As a matter of fact that is a common failure of CAs models, and for this example we committed this failure as well, because it is unavoidable.

Finally to calculate the new density for the whole federal state, the algorithm takes the sum of the old densities per federal state and divides it evenly on the new number of cells per state. E.g. if the density of Vienna initially has been 2 and the

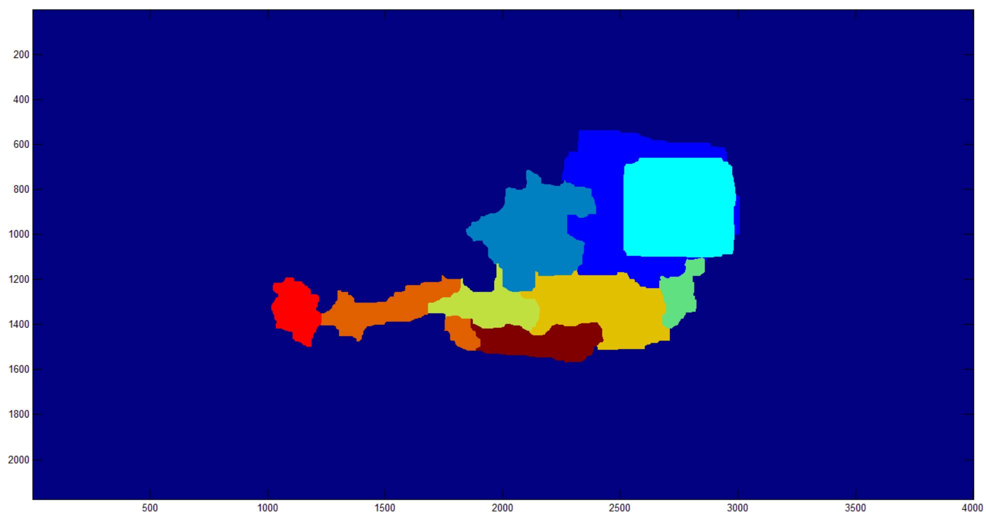


Figure 2.8: Comparison of Update Functions

number of cells was 8, the information stored in the 8 Vienna-value cells was of course 2. Let us consider Vienna has enlarged to 14 cells after a complete cycle of the CA Update algorithm then the new density value would be 8/7 = 1.41. These values will be saved for all cells representing Vienna at that moment. The algorithm then runs until the density is approximately the same everywhere, i.e. approximately be equal to 1. If we consider the population density question, we have seen the solution with von Neumann neighbourhood above, with Moore Neighbourhood we get:

The partial rectangular shape of the states is very well seen is a consequence of the Moore neighbourhood. We have seen the same effect producing diamonds with the von Neumann neighbourhood. The size ratios are similar to those of the Neumann-neighbourhood model. Again, it is the case that Lower Austria is no longer available around Vienna but disappeared in the lower right corner

As we have seen the first two approaches seem good in case of size of the federal states, but the update rules effect an unnatural form of the federal states, which is very different to a diffusion-based approach. So we tried a density-dependent "switch" mentioned above with a Neumann-neighbourhood. For each cell we do not automatically transform all adjacent cells with smaller values, but the

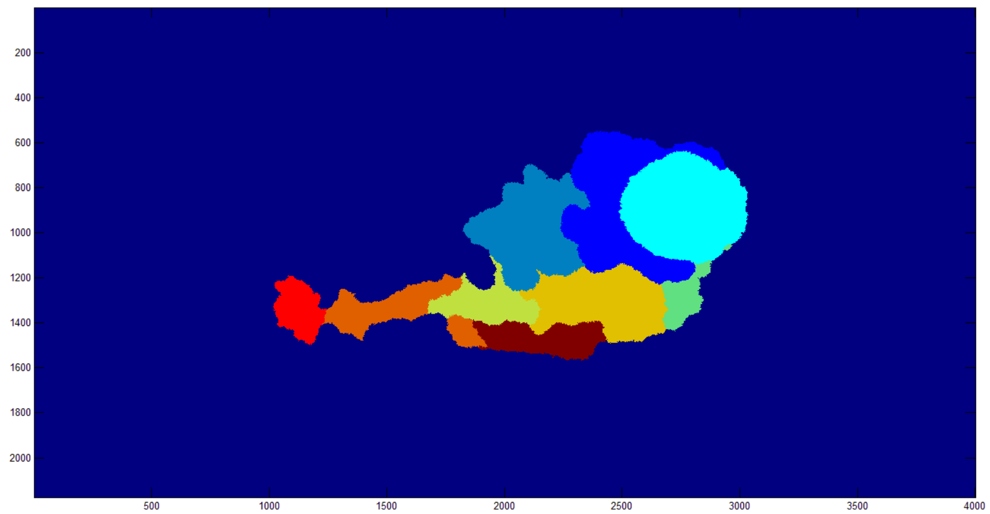


Figure 2.9: Comparison of Update Function „Switch"

algorithm decides by a combination of random number and on the difference between the two density values, whether the cell is taken over or not. If this difference is large, so is the probability that this cell is adopted as in the other two models. The smaller the difference, the less likely is the takeover of the adjacent cell. Specifically, the value will change if and only if the value of the cell is smaller than that of the consideration and the population value from the other cell divided by the population value of the cell considered is less than square of the 0-1 uniformly distributed random variable.

Neither a square nor a diamond: On this map we can see that on “visual validation” the City of Vienna shows the most realistic diffusion behaviour while inflating. On closer inspection we can see that the limits of Vienna are incorrectly frayed. The validation of our model is done by comparison with the already existing model, as there is no real system to be compared. Two aspects are very important for the comparison: size and shape and the boundary condition.

The validation of the size (1) is not very expensive. From the ratios of the countries before the application of the algorithm and the density values received by the algorithm, we can calculate the expected size. This can then be compared with the values that has been taken down the algorithm and specify the size of the country. We can also read out accuracy from the density values obtained at the end of the algorithm. The closer the values are to 1, the better is the result of the model. To visualise the validation of the size, we have created an error plot.

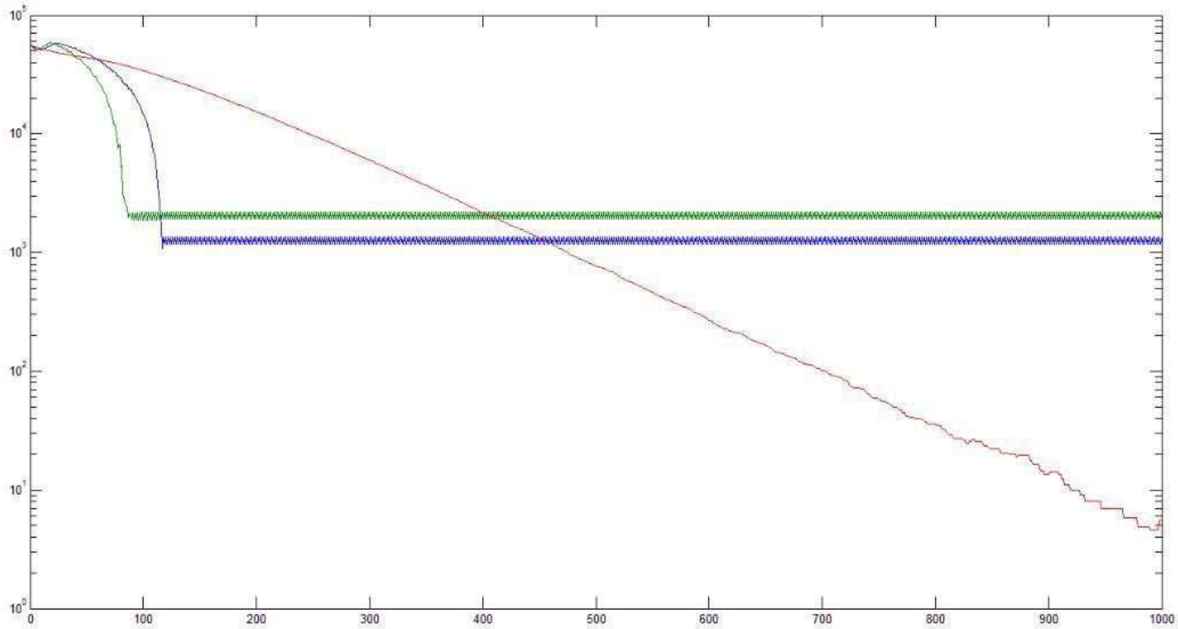


Figure 2.10: Error Plot

This plot shows the semi logarithmic error of the different models, i.e. the difference between the expected size and obtained size at the end of the algorithm for the federal states. The blue line shows the error of the model with Neumann neighbourhood, the green line shows the error of the model with Moore neighbourhood and the red line visualises the error of the model with the density-dependent "switch". We can see very well that the Neumann neighbourhood and the Moore neighbourhood have similar behaviour. After about 100 iterations below the error oscillates both models at 10^3 i.e. in total 1000 cells are mapped wrong on the whole map with 8,8 million cells.

The error oscillates, the same lower cells are transferred each step while they return again in the next step of the algorithm, because too many cells were overtaken. It can be seen that the algorithm with the Neumann neighbourhood starts oscillating a little later as the total number of cells overtaken is a little bit smaller than than with the Moore neighbourhood algorithm. However, by far the best result delivers the model with the density-dependent "switch" because here not all lower cells are overtaken during every iteration. Since the differences of density values are getting smaller every iteration also the probability that a cell is overtaken is getting lower. Therefore, this model can slowly approach to the correct result. But even this model starts oscillating slightly after iteration 1000. But concerning the total size it is clear that the model with density-dependent "switch" delivers the best results.

Turning now to the preservation of the shape of the boundary (2) when increasing or decreasing the provinces we already found that neither the model with Neumann neighbourhood model nor the model with Moore neighbourhood provides satisfying results. Here is a small example plot visualising the behaviour of a border shape using the Neumann neighbourhood:

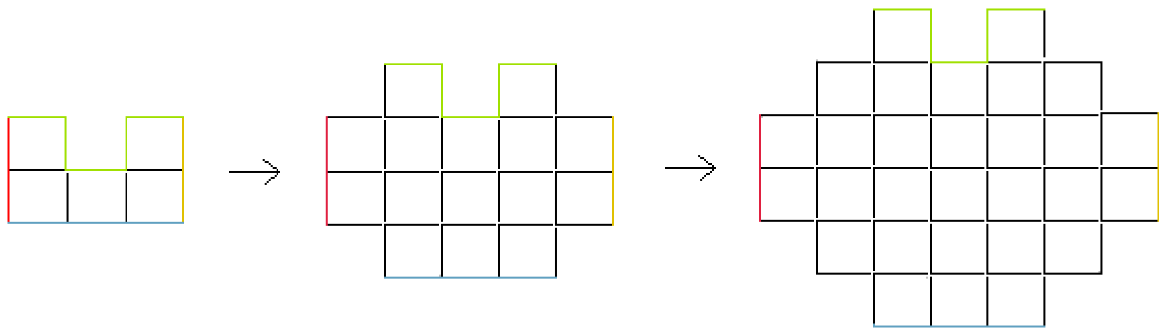


Figure 2.11: "Shape Maintenance with von Neumann Neighbourhood

This illustration shows that the original shape is maintained by the Neumann neighbourhood. As we can see, looking at the colour-coded limits, this neighbourhood is to maintain the shape of the boarders but does not enlarge it. When inflating this original boarder characteristic becomes smaller and the overall outline approaches to a diamond in any case, just according to the update rule and the von Neumann neighbourhood.

The example to the Moore neighbourhood with the same initial shape

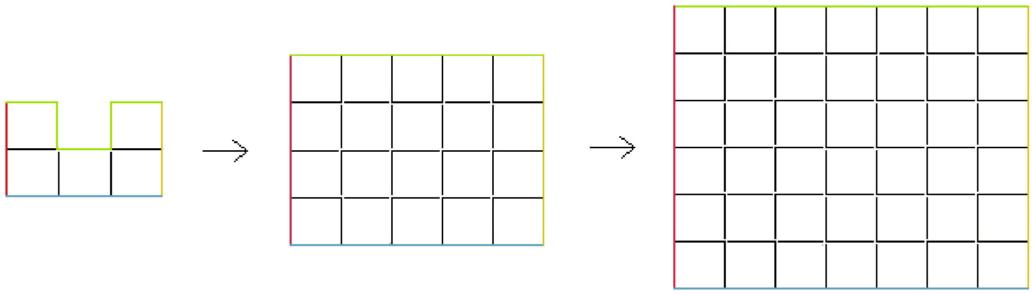


Figure 2.12: Squared Areas with Moore Neighbourhood

clearly shows that in this case, although a uniform magnification takes place,any minor unevenness is eliminated after a few time steps and the states get a rectangular shape. Looking at the model with the density-dependent "switch" the shape retention cannot be given to the original shape at the beginning. But this approach delivers the most naturalistic shape comparing to the original diffusion based approach. But as a matter of fact we don’t have mathematical formulation how this shape should look like. In summary it can be said that the shape of the resulting model is strongly coupled to model immanent rules and features of the CA. On the one hand retention with cellular automata is not possible. But at least the new size of the various provinces can be well approximated with cellular automata. Beside the basic ideas of developing new model approaches and problems and possibilities in comparing them, another effect can be clearly shown. As a matter of fact visual possibilities of models play an important role for users. For example the impact of tourism in Austrian provinces and their differences can be shown much more impressive than on a simple table.

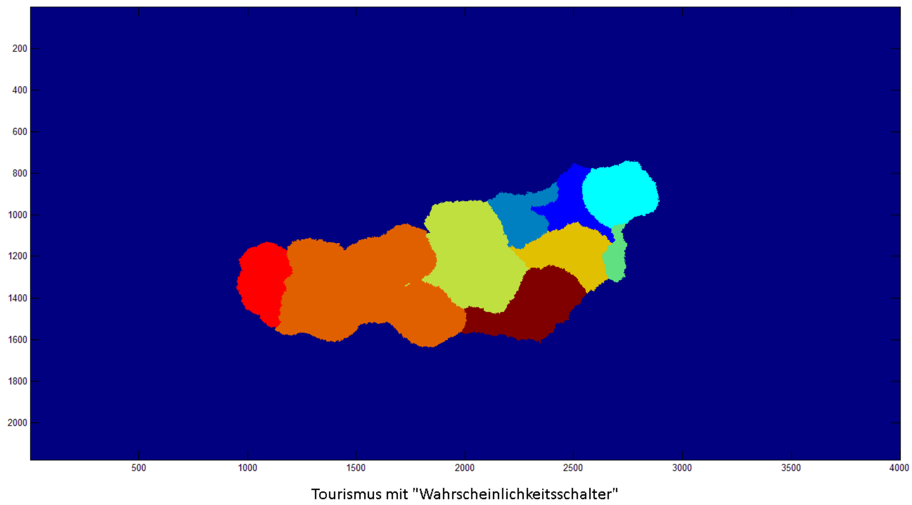


Figure 2.13: Application with Probability Switch

Concerning the over-night stays in tourism Tyrol is clearly Austria's "biggest" country. One last aspect of this approach is that it can be extended to other areas and maps very easy. E.g. in the case of European maps we can easily add Germanys map to the model and the computation of the diffusion process is automatically implemented by an increase of the matrices we use. Let us now consider Austria and Germany together in an international match. The algorithm starts from the normal map of both countries seen below.

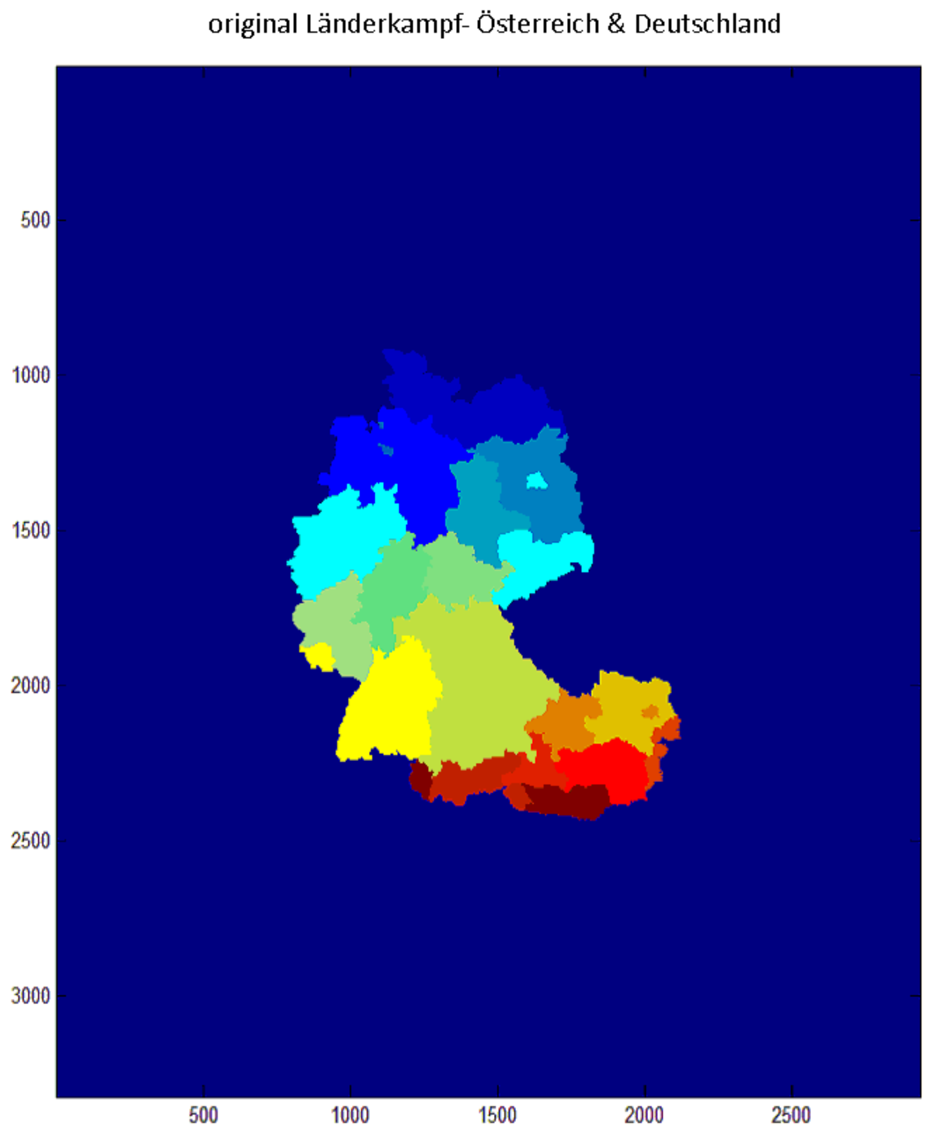


Figure 2.14: Comparison of Different Systems joined together

We now compute the comparison of wine-growing income from Germany and Austria for 2008, where Germany has [0, 0, 0, 0, 0, 1000, 55000, 0, 2000, 27000, 313000, 0, 6613000, 464000, 2518000, 9000] = [Schleswig Holstein, Mecklenburg-Western Pomerania, Lower Saxony, Hamburg, Bremen, Brandenburg, Saxony-Anhalt, Berlin, North Rhine Westphalia, Saxony, Hesse, Thuringia, Rhineland Palatinate, Bavaria, Baden Württemberg, Saarland]: Data Deutsches Weininstitut, 2008; in hectolitres and Austria has [1959308,800,21003,797038,100,214944, 200,100,220] = [Lower Austria, Upper Austria, Vienna, Burgenland, Salzburg, Styria, Tyrol, Vorarlberg, Carinthia]; Data Statistik Austria, 2008; in hectolitres

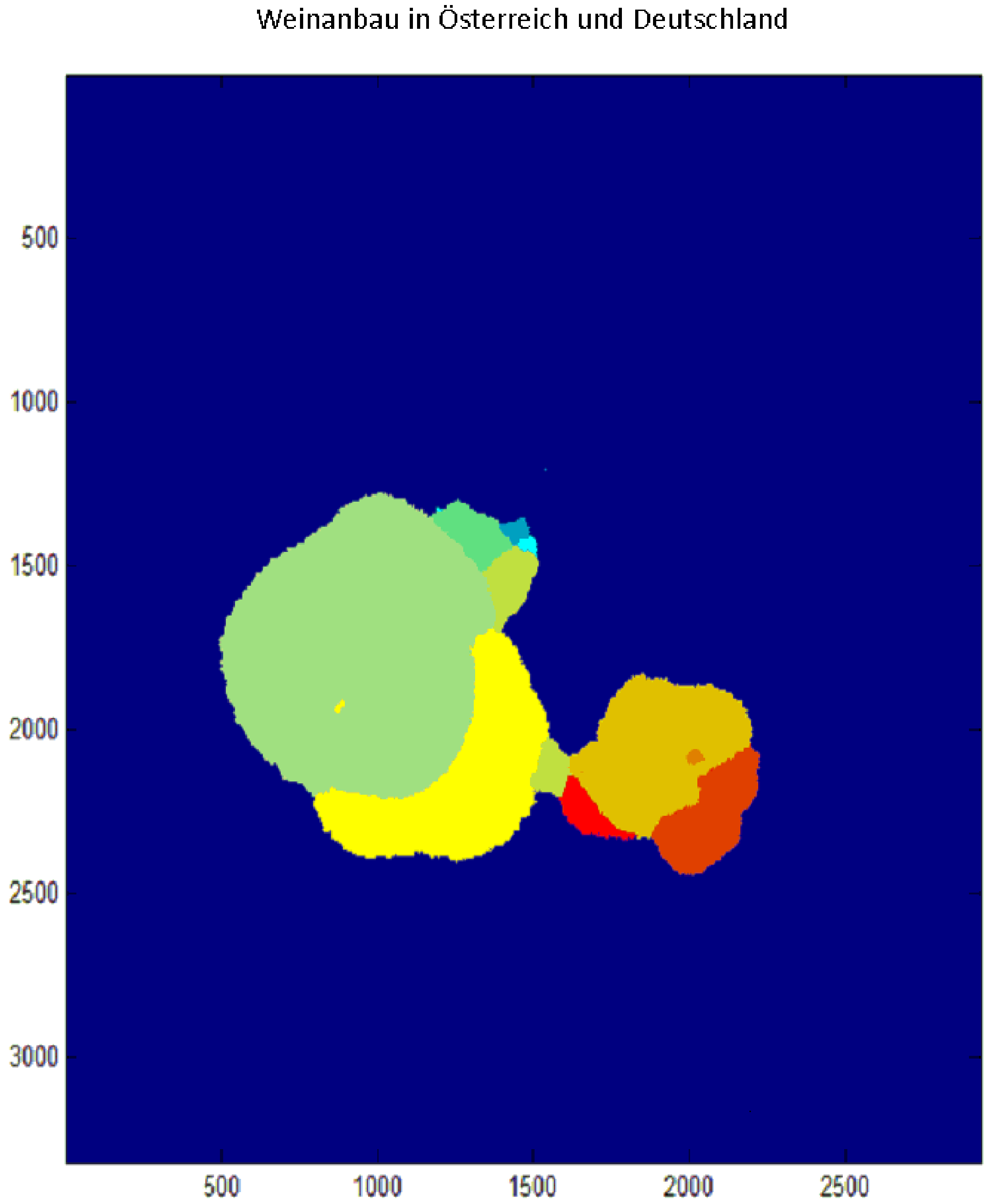


Figure 2.15: Comparison of Wine Production Germany and Austria

In Austria Burgenland, Lower Austria, Styria (in red) and Vienna resist vanishing in the diffusion process. Bavaria is split into two parts losing ground to the big wine producing German provinces.

A lot of such effects can be studied, but we do not present animation and implementation details in Matlab/Simulink. And besides such „interesting“ visual concepts, which we will focus on in a more serious way later in this work, we have learned the following things:

1. In principle at some point we have made a clear decision to introduce a „new model" instead of just using the same discrete approach as a simple implementation step. (When we decided to invent new rules for the CA update algorithm, instead the idea of following the mathematical description for discretisation). In this simple example we earned some problems in validating the second model later on. So the question we will have to discuss: is there a need or what is the benefit to generate another model? Later on we will see that be adding real world problems the question which of two models is the "correct" one will vanish and there might be occasions, where real life structures (or components of such structures) can be better implemented in one of the possible model approaches.
2. Comparison or "validation" between the two models was possible in case of the size of the system, i.e. do we get a correct density and total area of the analysed map, but it was not possible for "keeping" the shape of the various federal states. As a matter of fact until know we have not precisely defined what the "correct" shape would be. For cross model validation we will have to discuss rules what is the correct behaviour and why do we need this cross validation. In application areas (domains) like health system research we don't have e real system we could observe. So cross model validation is a promising approach.
3. As a side effect we have seen that the model approach clearly defines the results, as the neighbourhood definition pre-defines the shape of the provinces after they are inflated. This property of a modelling approach seems more or less obvious in this case (or can be seen easily as described), but we have the same problem for LGCAs, when dynamic movements persist in one direction producing artefacts, like spurious invariants in Lattice Boltzmann equations for fluid dynamics (Succi, 2001). In general we will see later, that every modelling approach generates model immanent behaviour which can by far be analysed in a better way, when we have the possibility to compare different model approaches. It helps to clearly separate between system immanent behaviour and (not intended) model immanent behaviour of simulations.

Our group analyses the problem that various modelling approaches are mathematically not well defined, but widely used. Besides, cellular automatons, there are to mention system dynamics or agent-based models (Einzinger, 2014). They share the situation, that these approaches do not have universally accepted mathematical definitions so it is necessary to give at least working definitions of both model types. In some cases and as the "best opportunity" we can integrate theories for two different modelling approaches in a theory on a higher level (parent theory). Einzinger showed this – on basis of two big research projects of our research group – for ABs and SDs by integrating them into general mathematical objects. Second we have to discuss the concept how we can transfer parameters from one model to another. Subsequently and third: is the presented CA just an implementation or another model? We will tackle this question in the next section:

2.2 Alternative Models and their Parametrisation

The following concepts are based on a publication first published by (Popper & Breitenecker, 2009a; Popper & Breitenecker, 2009b, Breitenecker & Popper 2004; Popper et al, 2006 and Miksch et al, 2015). The idea is that, based on the modelling process described, we can assume a parallel process of modelling and implementation. The keyword parallelisation is usually applied when speed is of essence. That normally means dividing the problem in such a way that parallel application of similar calculations allows for a quicker arrival at the result („*divide and conquer*"). In this case, the keyword „parallel" is, however, used to make a fundamental statement about the permutability of modelling and implementation while developing a mathematical model in general as well as about the specific implications this has for hybrid models that use different parallel or serial approaches to calculate a real system.

A mathematical model is developed in different stages. A model is first broadly designed, then placed in mathematical phrasing and then suitably implemented. These processes are not, as is usually assumed, utterly independent of each other, but must be considered interdependent. The way each is executed strongly influences the others.

As an example for the effects the stages of modelling have on the choice of relevant sets of parameters which do not only change in terms of numerical stability, but also reflect the structural differences of varying models of one and the same system. These considerations are of course particularly relevant regarding hybrid models. In our case, two or more models of the same real system are calculated in parallel or serially. Several cases must be considered: In the case of model approaches with similar structures, the parametrization follows the same sets of parameters. In a different case, the "permutation" of modelling and implementation described above renders different sets of parameters necessary. Using different model approaches that demand different parametrization leads to problems in validating and verifying the models. On the other hand, however, it also opens up new possibilities for the structural representation of real systems.

The development of modelling approaches that allow the calculation of simulations occurs via different stages. Classically, the problem is analysed, a model is designed, then phrased mathematically, implemented and finally identified. These stages are usually treated separately, isolated from the other stages and often – especially in larger scale modelling projects – they are worked on by different persons. While this was a sensible procedure with a view to a professional application of projects, it has led to the problem that these stages are now understood as in principle independent from each other.

Working on the *Argesim Comparisons* – a series of sample exercises on analysing modelling questions (Breitenecker et al, 2007) that are regularly published in the journal SNE (Simulation Notes Europe) –, the following question arose: Where does the aspect of modelling end and implementation begin? Take the following example: Discretisation of a differential equation means (leaving apart the modelling of the differential equation itself) that an existing exact model is replaced by a less exact but calculable "replacement". However, this step is in principle equivalent to the previous step of making assumptions in the process of modelling in order to be able to arrive at the differential equation itself in the first place.

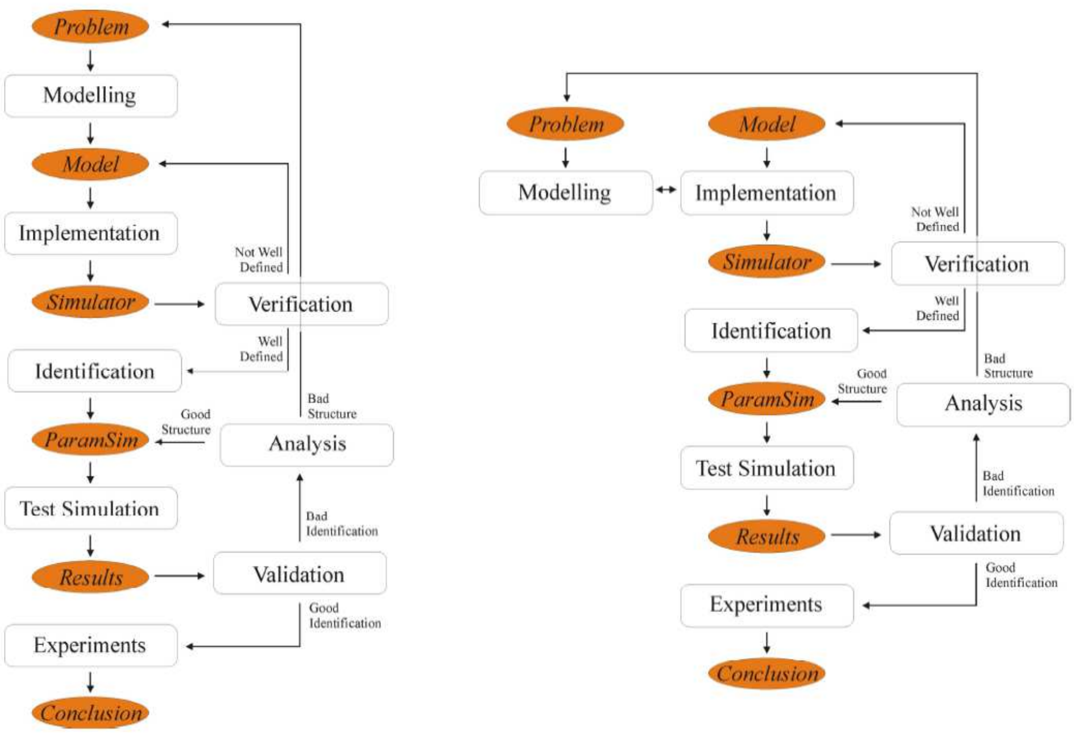


Figure 2.16: Depiction of the simulation cycle with the simplification of uniting the definition of a formal model and mathematical phrasing into a single step

While we can make exact statements on admissibility, area of validity and exactness of the result that is to be calculated thanks to brilliantly developed mathematical theories, this leads to a difference of the two stages in their application, but not in principle. More precisely, the fact that numerical computing has been established as an independent discipline while modelling has not makes the two stages different in how they can be practically solved but not in the problem they pose.

This principle is the same in both cases. Complexity is reduced in favour of usability of the resulting model. The important aspect of this thought is that the step of discretisation of a differential has a lasting effect on the behaviour and structure of the system model just as the assumptions made in the modelling process do. Specifically, each approach demands different parametrizations, which may differ drastically and thus strongly influence modelling and identification. This will be demonstrated at hand of an epidemic model. The problem of using such different approaches simultaneously in hybrid models (and the interface problems arising thereof) will be sketched out.

As described above, the choice of model influences the parametrization not only in terms of numerical stability or in potentially leading to problems in the eradication of state events that may arise. Its influence extends also to the quantifiability of parameters, *viz.* the connection between model structure and such quantifiability.

W. O. Kermack and A. G. McKendrick proposed in 1926 a simple SIR model for epidemic spread based upon a system of non-linear ordinary equations (Kermack & McKendrick, 1926). $S(t)$ is the number of susceptible individuals, $I(t)$ the number of infected individuals and $R(t)$ the number of recovered individuals, at time t respectively. $S'(t)$, $I'(t)$ and $R'(t)$ represent the change of susceptible, infected and resistant individuals. The amount of susceptible individuals that become infected is described as $\gamma S(t)I(t)$, where γ is referred to as infection rate. The amount of infected individuals that become resistant is described as $\delta I(t)$, and δ is named recovery rate. Since the number of individuals in our system shall be constant, these growth terms yield the following system of ordinary differential equations (ODE):

$$\begin{aligned} S'(t) &= -\gamma \cdot S(t) \cdot I(t) \\ I'(t) &= \gamma \cdot S(t) \cdot I(t) - \delta \cdot I(t) \\ R'(t) &= \delta \cdot I(t) \end{aligned} \qquad 2.1$$

This classical ODE model does not reflect any spatial distribution. The spread and recovery of an infection can be interpreted as a diffusion process among particles (= peoples). Therefore, a lattice gas cellular automaton (LGCA) can be considered as describing the epidemic. LGCA are two-dimensional cellular automata with particles moving from cell to cell during each time-step of the automata. We have to distinguish between the HPP (Hardy, de Pazzis, Pomeau, 1973) and the FHP (Frisch, Hasslacher, Pomeau, 1986) model. The FHP model consists of a hexagonal structure containing a maximum of six particles per cell again being defined by its lattice-vectors connecting the cell to its six nearest neighbours. Especially with a hexagonal lattice, LGCA are used for simulating the movement of gas particles or fluids.

We will additionally allow particles to take one of the states susceptible, infected or recovered in order to simulate the spatial spread of a SIR-type disease.

Accordingly, we assume that our cells are arranged on a two-dimensional hexagonal grid structure and represent a spatial segment. Each cell can hold at most six individuals. Each individual is in one of the three states susceptible, infected or recovered. Contacts happen pairwise between all individuals which are located in the same cell at the same time. To simulate a mixture of the individuals, they move around the cells in random directions (diffusion) or as defined by the FHP-I collision rules [5]:

- The position of an individual within a cell defines its moving direction (Figure 2.17).
- After the movement phase a collision phase (Figure 2.18) takes place. The FHP-I variant only defines special two and three particle collisions. All other collisions happen without any change of moving direction. When two individuals collide as in Figure 2.18, they are reflected clockwise or counter clockwise with probability 0.5. When three particles collide as pictured in Figure 2.18, then they are reflected clockwise.

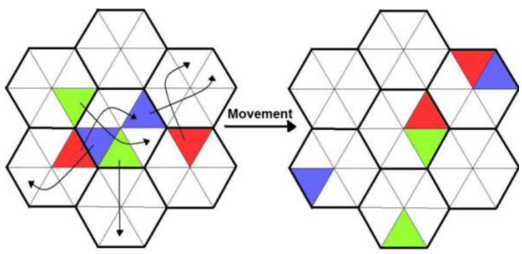


Figure 2.17:Schematic visualization of LGCA movement rules

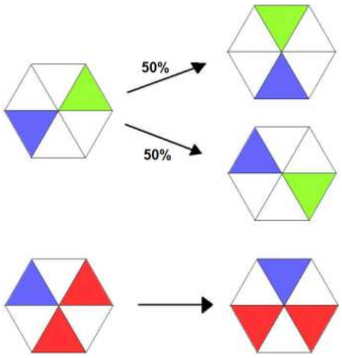


Figure 2.18: FHP-I collision rules.

When a susceptible individual meets an infected individual within a cell, it shall become infected with probability φ. An infected individual recovers with probability ϕ.

With a first approach the models can be compared and by showing (under certain assumptions) the equivalence of the models quantity can be described. Simulation with the ODE model can be compared with the results of the LGCA model. For this comparison, adequate parameters and spatial distributions have to be chosen. As we chose parameters for the ODE system (Table 2.1) we can try to simply use parameters for population sizes in the LGCA model and infection and recovery rates.

$S(t{=}0) = S_0$	16000
$I(t{=}0) = I_0$	100
$R(t{=}0) = R_0$	0
Infection rate γ	$0.6{\cdot}10^4$
Recovery rate δ	0.2

Table 2.1: initial values and parameters for comparison of ODE and LGCA model

A FHP LGCA with a domain size of 100×100 (and therefore 10^4 hexagons), with infection rate of γ = 0.6 and periodic boundary conditions to remodel the system was implemented (as initial configuration, uniformly distributed individuals of type S and I were chosen).

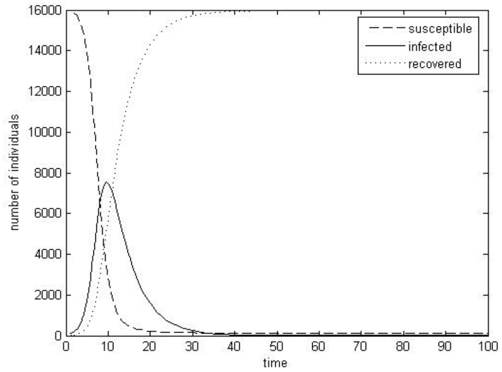


Figure 2.19: Simulation results for ODE model

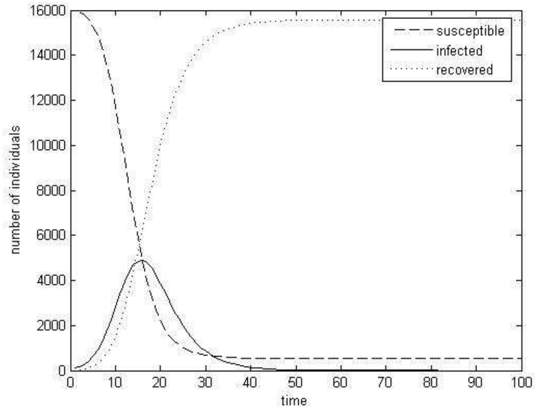


Figure 2.20: Simulation results for FHP LGCA model

However, the results show the problems of parameter identification, as the presented results (Figure 2.19 and 2.20) are of similar qualitative nature but differ quantitatively for the different approaches. One reason for this is the fact that infected individuals form spatial groupings in the LGCA and thus slow down the speed of the epidemic. This can be described as a structural difference as we have homogeneous behaviour on the one hand and inhomogeneous behaviour on the other, where infection occurs within one cell of the automaton, rendering the infection probability much lower as no more than a few individuals can "meet" in one cell.

This structural problem can be solved ostensibly. For lattice Boltzmann cellular automata it can be shown that the averaging states converge under certain circumstances to solution of the continuous Boltzmann equation. For the investigated LGCAs, a kind of "convergence" can be shown experimentally. The idea is to prevent clustering in the LCGA and observe again the average states, ensuring perfectly uniform distributions for all three groups of populations (*S(t), I(t), R(t)*) by randomly rearranging all individuals in every time step of the automaton.

However, the "interdependence" of model structure and parametrization should be entirely resolved. On the one hand, it soon becomes evident that population size and raster size are directly interdependent and have a direct impact on the quantitative results of the model. On the other hand, one can see that the infection and recovery rates directly react to the resultant concentration. These relationships are manageable in this model, which was consciously chosen for its simplicity. For doing so two steps were taken by the author together with F. Miksch, C. Haim, G. Schneckenreither (Miksch. Popper et al, 2015) . On the one hand an abstract model was developed, which is the „parent" model for both models described above.

Let N be the number of individuals of the population. The population can neither be joined nor left by individuals, which means that N is a constant number. Each individual shall be in one of the states susceptible, infected or recovered. The system evolves by discrete steps of one time unit and the spread of the disease is characterised by contacts between individuals, transmission of the disease and recoveries.

Each individual is assumed to have an average of C contacts per time step; these contacts always happen between two random individuals. Since the discrete time steps are atomic by definition, the order of contacts is irrelevant. However, in order to ensure that susceptible individuals cannot get infected and infect others simultaneously, the infection-states of the individuals change after all contacts have been processed according to the following paradigms:

- When a susceptible individual gets into contact with an infected individual, the susceptible individual becomes infected with probability α. This probability applies for each contact separately.
- Infected individuals recover at the end of each time unit with probability β.
- Recovered individuals always remain recovered.

Parameter	Description
S_0	initial number of susceptible
I_0	initial number of infected
R_0	initial number of recovered
C	contacts
α	infection probability
β	recovery probability

Table 2.2. *System Parameters*

As a direct result we can now describe the parametrisation for both models as follows:

Before setting the ODE parameters, we need to deal with the follwing concern. An ODE $A'(t) = -\xi A(t)$ with $0 \leq \xi \leq 1$ represents a system where A is continuously decreased. However, ξ does not represent the amount of decrease within one time unit. If A should be decrease to $\hat{\xi} \cdot A$ within one time unit, then ξ needs to be set as

$$\xi = \ln(1 - \hat{\xi}). \qquad 2.2$$

This is based on the fact that the general solution of the ODE is $A(t) = A(0) \cdot e^{-\xi t}$. The condition that A should be decreased leads to the equation $A(t+1)$=$(1 - \hat{\xi}) \cdot A(t)$, and further results in the formula above.

Identification of the infection term $\gamma \cdot S(t) \cdot I(t)$ takes a look at a single individual, which has C contacts per time unit in average. Among the contacts, it has $C \cdot \frac{I}{N}$ contacts with infected individuals. Each contact causes a transmission with probability α. The transmissions are statistically independent events. Hence, the infection probability per time unit is computed as the probability to get infected at least once, which is represented by the formula $1 - (1 - \alpha)^{C \cdot \frac{I}{N}}$. Considering Equation (4), the infections in the ODE are represented by $-\ln\left(1 - 1 + (1 - \alpha)^{C \cdot \frac{I}{N}}\right) \cdot S$, which can be rewritten as $-I \cdot S \cdot \frac{C}{N} \cdot \ln(1 - \alpha)$. Hence, γ is identified with $-\frac{C}{N} \cdot \ln(1 - \alpha)$. Since the recovery rate δ determines the fraction of infected individuals that recover during one time unit, δ calculates as $-\ln(1 - \beta)$.

The identified parameters are summarised in Table 2.3.

Parameter	Identification
$\boldsymbol{S(0)}$	S_0
$\boldsymbol{I(0)}$	I_0
$\boldsymbol{R(0)}$	R_0
$\boldsymbol{\gamma}$	$-\frac{C}{N} \cdot \ln(1 - \alpha)$
$\boldsymbol{\delta}$	$-\ln(1 - \beta)$

Table 2.3. *Parameter identification of the differential equation model.*

For the LGCA we get the following: The size of the LGCA plays as described above an important role because it affects the density of particles and thus the number of contacts. For the sake of simplicity, we use a grid with $width = length = n$ and accordingly n^2 cells with six places each. Table 2.4 shows the parameters of the model with appropriate parameterisation. For a given number of individuals, the number of contacts depends on the size n of the LGCA.

The correct identification for n is crucial, but follows a simple calculation: Assuming a uniform distribution of the individuals, each of the six slots of a cell is occupied with the same probability. For a given individual there are 5 unoccupied slots in the same cell. Accordingly $N-1$ remaining individuals occupy $6n^2-1$ remaining slots and the individual has an expected number of

$$C = 5 \cdot \frac{N-1}{6n^2-1} \qquad 2.3$$

contacts within this cell. Adjusting n, which has to be an integer, to meet a given number of contacts leads to the identification in Table 4.

Parameter	Identification
$\boldsymbol{S(0)}$	S_0
$\boldsymbol{I(0)}$	I_0
$\boldsymbol{R(0)}$	R_0
$\boldsymbol{\varphi}$	α
$\boldsymbol{\phi}$	β
$\boldsymbol{n}$	$\left\lfloor \sqrt{\frac{5(N-1)+C}{6C}} \right\rfloor$

Table 2.4. *Parameter identification of the cellular automaton model.*

By doing so finally we get a analytic „Conversion" rule for parameters for both models. There is a strong analytical relation between the ODE approach and the CA model.

For the infections the following calculation aims to estimate the number of new infections in a time step in the LGCA. Consider a susceptible individual in a cell (only susceptible individuals can get infected). Then there are altogether $6n^2-1$ remaining slots in the LGCA, 5 remaining slots in the cell and I infected individuals. Define the probability of i slots in the cell being occupied by infected individuals as q_i. Under the assumption that the individuals are uniformly distributed, the number of infected individuals in this cell is distributed according to a hypergeometric distribution. The probabilities calculate as choosing i out of I infected individuals on 5 out of $6n^2-1$ places:

$$q_i = \frac{\binom{5}{i}\binom{(6n^2-1)-5}{I-i}}{\binom{6n^2-1}{I}}, \quad i = 0 \dots 5 \qquad 2.4$$

The expected value E of this hypergeometric distribution is

$$E = \sum_{i=0}^{5} q_i i = I \frac{5}{6n^2-1}. \qquad 2.5$$

Using the identification in $C = 5 \cdot \frac{N-1}{6n^2-1}$, the expected value can be written as

$$E = I \frac{C}{N-1}. \qquad 2.6$$

With these preparations the actual infection probability of a susceptible individual can be calculated. If the cell is occupied by i infected individuals the probability for an infection of the susceptible individual is $1-(1-\alpha)^i$. Hence the expected probability for an infection is $\sum_{i=0}^{5} q_i(1-(1-\alpha)^i)$. Considering the first two terms of the Taylor series expansion at $\alpha = 0$ and the identification in $E = I\frac{C}{N-1}$. leads to the following approximation for this probability.

$$\begin{aligned}\sum_{i=0}^{5} q_i\left(1-(1-\alpha)^i\right) &\approx \sum_{i=0}^{5} q_i i\alpha = \\ = \alpha \sum_{i=0}^{5} q_i i \ &= \alpha E = \ \alpha I \frac{C}{N-1}\end{aligned} \qquad 2.7$$

Multiplying this with the total number of susceptible individuals leads to $S\alpha I \frac{C}{N-1}$ as an approximation for the expected total number of new infections for one time unit in the LGCA for small values of α.

The term in the ODE for infections of one time unit per susceptible is computed as $1-(1-\alpha)^{\frac{C\cdot I}{N}}$. In the term for the CA, $\frac{I}{N-1}$ can be approximated with $\frac{I}{N}$. Natural limitations are $\frac{I}{N} \leq 1$ and $C \leq 5$. For small α and the natural limitations, $1-(1-\alpha)^{\frac{C\cdot I}{N}}$ is an approximation of $\alpha\frac{C\cdot I}{N}$.

For recoveries an infected individual in the LGCA recovers during one time unit with probability β, hence the expected amount of infected individuals who regenerate in one time unit is βI. The same factor also occurs in the differential equation and Table 2.3 as $-\ln(1-\beta)$.

For further development of the modelling approach see (Bicher & Popper, 2013), where additionally an Agent Based Model was developed. Based on this new hybrid modelling methods mixing agent-based and differential equation modelling are developed, on the one hand utilizing the great flexibility of time discrete microscopic models and on the other hand getting benefit from the fast computation properties and good numerical methods for differential equations.

2.3 Summary

We have solved – for a concrete example - the transfer of one model to another model. The parameters could be analytically transferred from one model. We have learned that there is the possibility to define a „parent model" mathematical system, which represents the reality (or a problem defined on the reality) quite good. From this point we could develop two equivalent models. But still there are many questions open. The two models are identical in terms of basic „structure" (all defined characteristics were modelled, and in terms of parameters. But still the behaviour of the models are different, as immanent the one solution models he spatial effects of an infectious disease the other one doesn`t. And second the ODE model can be interpreted as the model and the CA can be seen as implementation of the first one. But why do we have aspects described above, which are „additional" to the given ODE model?

Last but not least we tried to introduce interventions into the system – from the model point of view a new „question" was introduced, and the model was screwed a little further. As a formal description it was sufficient to „test two models against each other", but for real life application probably these kind of vaccinations wouldn't be able to realize the questions and goals described in Chapter 1.3.2.

In Chapter 3 we will focus on the „improvement" of the modelling circle in terms of

- In Chapter 3.1 we want to have a look on how do we get the problem definition of our domain, if system boundaries and/or research questions are changing via improvement of complexity

- What additional steps are needed to make models comparable in terms of their usability to fulfil needs in modelling well defined problems in Chapter 3.2
- What concepts do we need to couple models to fulfil future complex processes, e.g. multi-method modelling in Chapter 3.3
- And what aspects have to be obeyed, when modelling concepts should be transferred between different domains. An example for a layout will be shown in chapter 3.4

3 Improving the Modelling Process

3.1 Data – System Knowledge – Question of Research

To match complex modelling needs, various changes on the given modelling circle have to be implemented. We will see later, that formal definitions for comparison of models are needed. Secondly coupling of simulation approaches need to be improved. So the modelling circle seen in Chapter 2 has to be extended as follows:

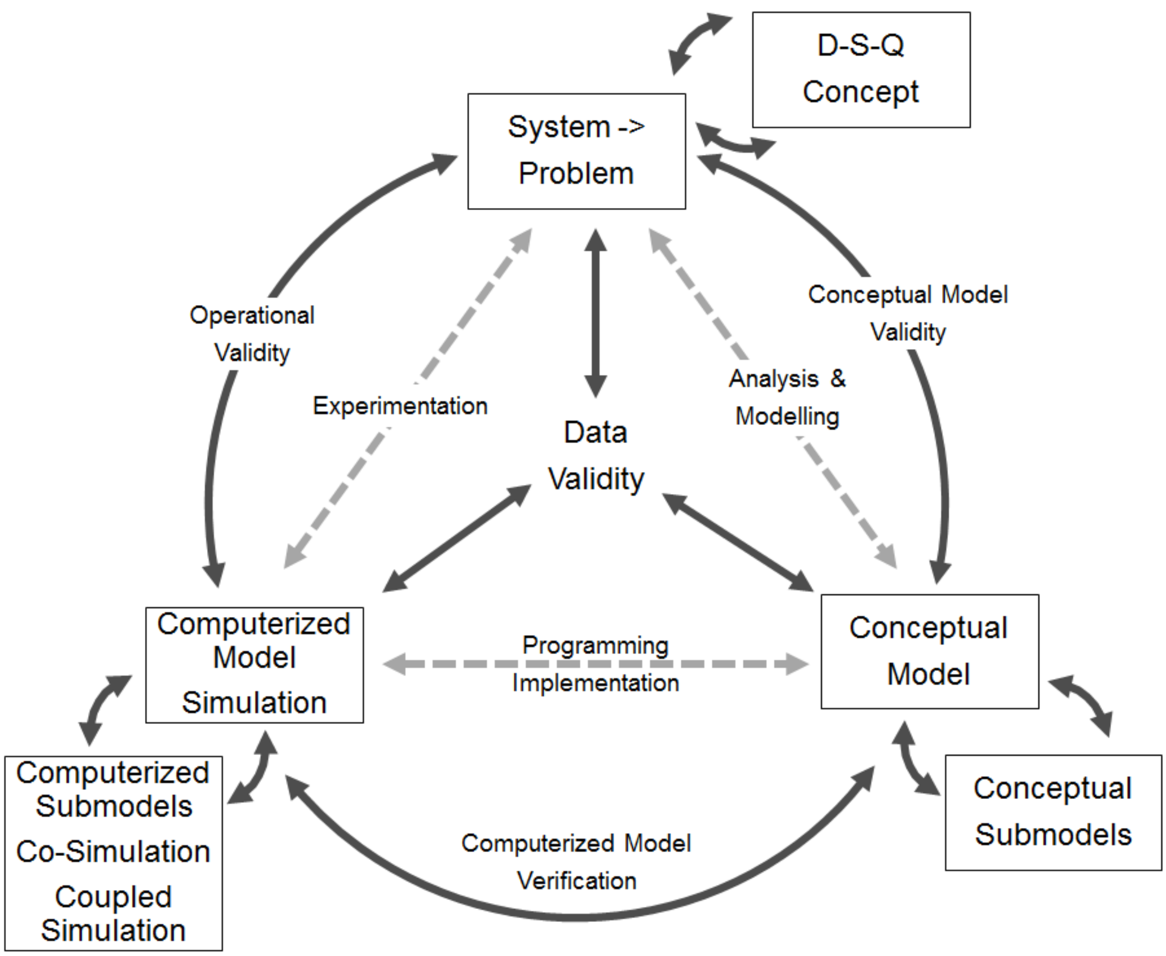


Figure 3.1: Revised Modelling Circle

The additional tasks and resulting needs can be seen in all areas of the modelling circle. Conceptual alternative models and sub models need additional formalisation concepts and tools for conceptual model validation. For implementation the definition of sub models of computerized models will need both, definition of various coupling modes as well as concepts for implementation. But the first step is a change in the definition of the formalised system and later on the problem. The D-S-Q Concept was developed over the last years, according to the needs of "real life projects". As first step the concept of identification of the physical system to the mathematical system was sharpened by economical needs and contains the following steps:

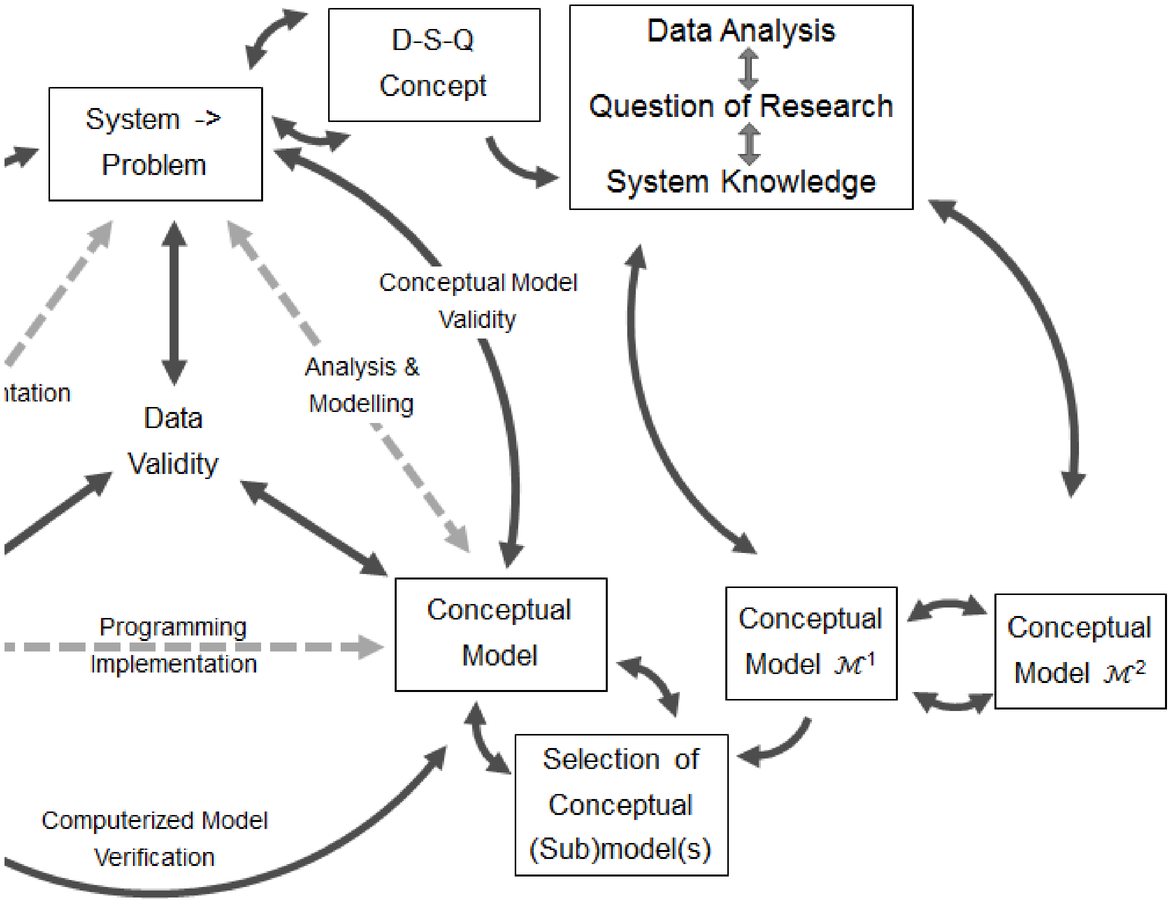
- Data Analysis
- System Knowledge
- Question of Research

Of course all the mentioned steps itself are well known and should be executed. Nevertheless the naming of a "concept" shall underline existing deficiencies in the formalisation of this process.

In most cases identification of which model concept to choose is mainly affected by domain immanent dominance of methods, e.g. given usage of Markov models within the area of clinical data analysis. By defining a "concept" the emphasis shall be laid on the change from a method driven approach to the D-S-Q approach.

According to the system we look at a problem and a research question may occur. There are diverse standards how these questions have to be formulated, like in health economics and evidence based medicine the PICO standard is state of the art (Gerber 2006). After doing so availability of data has to be checked. Depending on the defined research question necessary quality and types of data may vary in a wide range. So a basic idea, which modelling concept shall be chosen is defined. After doing so according to all information collected so far, the analysis of the system knowledge is done. According to engineering, this step seems easy, but regarding "black box" domains this is one of the most important steps, as normally no dynamic modelling is domain immanent established. After doing the first iteration of this process the whole process has to be repeated until (1) a sufficient modelling concept is developed or (2) the modelling approach as tool for decision support is disqualified in this case. This exclusion is one of the most important results of the D-S-Q process, as already in an early phase of a project it has to be decided, whether the research question can be analysed via dynamic modelling or not. Normally this is not resulting because of one of the three explored points, but it is a combined, emerging effect and a result of the iterative process.

The basic idea resulted from economic needs. As a matter of fact when simulation projects should be implemented in "non-modelling-domains", there is an urgent need to prove the effectiveness and feasibility of the planned project. Budget should not be invested without a more or less reliable chance of reaching the targeted goal. So the planned model is tested right at the beginning and the effort should not exceed 5-8% of the planned total costs of the simulation project. Further investigations are in progress.



In chapter 3.2. we will see what is needed to do better comparison of models, chapter 3.3. will address the question of coupling of models to solve complex systems which are divided in heterogonous subsystems and last but least in chapter 3.4 an example the for a concept to transfer a modelling approach to another domain for modelling rising complexity of the given system will be presented.

3.2 Comparison of Models

In previous chapters we have seen, that in principle different modelling concepts can be compared and transferred under certain circumstances. But still we lack in a reproducible approach to compare different models. As we have seen in chapter 2 cellular automatons are a well-established and beneficial modelling approach for various domains and research questions. But for further analysis a mathematical conception is missing. „Models can be created with just an intuitive understanding of the underlying modelling method, but this comes with the disadvantage that rigorous mathematical statements about methods are then impossible. These statements require that models and systems are defined as mathematical objects, rooted ultimately in an axiomatic system such as set theory." (Einzinger, 2014) So we will have as an example a closer look on the mentioned cellular Automatons.

3.2.1 Formal Definition of Cellular Automatons

The classical concept of cellular automatons was compared to other modelling approaches in chapter 2.1 and 2.2. Questions like quantitative comparison and transfer of parameters were solved sufficiently (in examples). But to go further it will be important to find definitions for comparing modelling approaches on a mathematical basis. CAs are an automaton based description upon a discretisation of space and time. Each cell can hold a finite number of states and the temporal evolution of the automaton is governed by transition rules, which act locally and simultaneously on the cells. The transition rules can either be deterministic or probabilistic. Locality is introduced by a neighbourhood function which defines the cells being determinant for influencing the cell state. The transition rules are purely deterministic but will not be presented here in detail. As described earlier there exist many generalisations of cellular automata models. Among them, lattice gas cellular automata (LGCA) and Lattice Boltzmann cellular automata (LBCA) allow to model streaming (Navier-Stokes) processes between the cells of the automaton.

In literature different approaches to define CAs can be found. They normally have the following characteristics in common:

- regular alignment
- passive containers for states
- unique update function
- regular neighbourhoods

which we use as basis for a formalism, that we call "least common formalism". Günther Schneckenreither presented such formalism in his thesis (Schneckenreither, 2014), which I was honoured to co-supervise. It can be summarized as follows:

Initially we regard cells as abstract entities of a set M. Additionally there usually exists a "topological" alignment of the cells in M, which can be formalised through a bijective mapping

$$\mathcal{I}: M \leftrightarrow I, \text{ where } I \text{ is a certain connected set of indices in } Z^d.$$

For every cell the mapping $N: M \rightarrow M^k$ defines a collection of neighbouring cells. we call $N(m) = (n_1, \dots, n_k)$ the neighbourhood of m. if there exists a mapping $\mathcal{I}$ as defined above, then N usually can be written as

$$N(m) = \left(I^{-1}(I(m) + j_1), \dots, I^{-1}(I(m) + j_k) \right)$$

where $J := (j_1, \dots, j_k)$ is a tuple of "relative" indices in Z^d. The neighbourhoods of all cells also imply a "topological" structure on M. Since for some cells $I(m) + j_l$ may not lie in the domain of I^{-1}, these "boundary conditions" must be treated separately. For further information see (Schneckenreither, 2014).

Every cell takes a state from a set of possible states S, accordingly there exists a mapping $\mathcal{S}: M \to S$ which assigns a state to every cell. Except for boundary conditions, the states of the cells are iterated in the following way

$$\mathrm{E}: \mathrm{S}^{\mathrm{M}} \to \mathrm{S}^{\mathrm{M}}: \mathcal{S}_t \to \mathcal{S}_{t+1}$$

with

$$\begin{aligned} \mathcal{S}_{t+1(m)} &= f\ o\ (\mathcal{S}_t)^{(k)} oN(m) \\ &= f\ o\ (\mathcal{S}_t)^{(k)}\ \left(I^{-1}(I(m) + j_1), \dots, I^{-1}(I(m) + j_k) \right) for\ all\ m\ in\ M \end{aligned}$$

where $f: S^k \to S$ is the (unique) mapping that calculates a new state for a given tuple of (neighbouring) states. Finally we define (ordinary) cellular automata as tuples $\left((M, I, \mathcal{I}), J, S, f\right)$

Based on this concept of a formal definition, extended concepts of cellular automata are very easy to define. As mentioned earlier the cells m in M are aligned through the index set I and the mapping $\mathcal{I}$ we can define unaligned cellular automata which lack such an alignment. In this case the mapping $N: M \to M^k$ must be explicitly defined and we can use the tuple representation (M, N, S, f) compared to $\left((M, I, \mathcal{I}), J, S, f\right)$.

Definition 4.1 (Cellular Automaton)**.** A Cellular Automaton is a tuple (M, N, S, f), where M is a set of entities, N is a mapping function, S is a set of possible states and f is an update function.

This conception of cellular automata can be regarded as being closely related to agent-based systems because the neighbourhood structure is more a network than a grid. However not only the topological structure of our basic definition can be modified as shown, we may also regard various types of states. As an important example we can take stochastic states. Cells can take states with a certain probability distribution, on the other hand restriction to discrete states can be achieved by setting $S = \{1, \dots, r\}$. Elementary cellular automata [Wolfram] are defined by $S = \{0,1\}, I = \{1, .., n\}$ and one of $2^{2^3} = 256$ possible update functions $f: \{0,1\}^3 \to \{0,1\}$. more complex approaches like lattice gas cellular automata or the lattice boltzmann method can be interpreted with state spaces $S = \{0,1\}^6 or\ S = R^8_{\{+\}}$ etc.

As an important point, and for the sake of comparability to literature, most definitions and conceptions in literature are covered by the formalism described above. From this "stating point" it is – as described – possible to reduce the possibilities and also reduce the mathematical complexity of the formalism to "match" with a given CA. On the other hand the characteristics can be extended for all aspects of the CA (alignment of cells, neighbourhood, states, update function). For further reading I refer to (Schneckenreither, 2014) e.g. for a general approach for modelling or approximating certain types of continuous systems using cellular automata, where he defines (locally characterised) evolution systems using the paradigms of cellular automata, and shows possibilities for investigation of linear evolution equations and parabolic differential equations in this context.

3.2.2 Agent Based Models Formal Definition & Analytic Analysis

In the section above the connection of cellular automatons to agent based models was mentioned. To take a further look on it, we have to discuss the concept of agents in a little more detail. In 1971 economist Thomas C. Schelling published his attempts to model the dynamic behaviour of racial segregation in society (Thomas C. Schelling, 1971). These attempts shared the main idea that a population, divided into two or more racial concurring subpopulations, is initially distributed randomly onto a two dimensional rectangular spatial grid, as it was already used before in most cellular automata introduced by e.g. Ulam or Von Neumann. Hence each individual (or clusters of individuals) inhabits exactly one site on the grid. After the initial setup each individual dynamically either decides to remain at the current site or to move away due to an "unpleasant" neighbourhood.

Although the research question behind Schelling's models seem very doubtful from our current point of view, yet these models claimed a big amount of fame due to their big influence on a novel modelling approach: agent-based modelling. While Turing's state machines (Turing, 1950) and Von Neumann and Ulam's cellular automata (Neumann, 1966) were based on the idea that one underlying machine (the Turing-machine respectively the automaton itself) decides about the progress of all states of the system at once, Schelling initiated to think about shifting this responsibility to the microscopic parts of the model, in this case the individuals. This can be seen picking some phrases in his work: Each individual "moves" to a site depending on its "own neighbourhood". Hence the inhabiting site can rather be seen to be a state of an individual, than the individual is a property of the inhabiting site, which would be the standard interpretation in a cellular automaton. We can see here the corresponding concepts to Luhmann described in chapter 1.

Based on these ideas Schelling's models are in literature often denoted as the first agent-based models. As the shift of responsibility for the update of the state, from the underlying automaton to the individuals, combined with constantly increasing computational resources, created an immense space of freedom for adaptions and further development of the modelling method, it has become more and more difficult to find a proper definition summarising all models developed this way.

Nowadays one possible attempt to define agent-based modelling can be found in (Macal and North 2010). The definition was developed within a tutorial during the 2005/06 Wintersimulation Conference and rather poses for a brief summary of necessary characteristics of agent-based models than a classic mathematical definition.

According to Macal and North (2010), an agent-based model or system typically consists of three parts:

- The agents of the system with all their properties and their behaviour.
- Interactions and relationships (e.g., through a connection network) between the agents.
- An environment where the agents live and with whom they interact.

The agents are of course a necessary component of every agent-based model. Additionally, an agent-based model without some kind of interaction between the agents would not have any advantage over simulating each agent individually, such as in a microsimulation model. Agents without an environment (e.g., an underlying space) are, on the other hand, imaginable.

On the most basic level, an agent is at least an object, because it has both attributes and behaviour (North & Macal, 2007). This shows the strong relationship with objects in object-oriented programming, where the attributes of an object are its fields (variables) and the behaviour are its methods (functions). Therefore, it is natural that most implementations of agent-based models use object-oriented programming. (D'Inverno and Luck, 2004) propose the framework SMART for agency, which consists of a hierarchy of the terms

1. Entity
2. Object
3. Agent
4. Autonomous Agent

Each term has one additional definition compared to the preceding term. Entities are just a collection of attributes. Objects, as stated above, have also behaviour, agents have goals, and autonomous agents have motivations; they "pursue their own agendas as opposed to functioning under the control of another agent" (d'Inverno & Luck, 2004). All objects are entities, all agents are objects, and all autonomous agents are of course agents.

According to Macal and North (2010), the five following characteristics are stated to distinguish agent-based modelling from all other modelling approaches. A model consisting of a number of microscopic parts, furthermore called agents, is called an agent-based model, if all agents …

- are uniquely identifiable during the whole simulation.
- act autonomous and independent.
- inhabit a common environment and can communicate (interact) with it and each other.
- act targeted (goal oriented).
- can adapt their behaviour (learn).

There are several other characteristisation of agents in the literature. (Wooldridge, 1997), for example, requires the following four properties:

- Autonomy: Agents have their own encapsulated state that is not directly accessible to other agents, and they can decide on their own actions.
- Reactivity: Agents live in an environment, which they can perceive and where they can take actions to react to changes in this environment.
- Pro-activeness: Agents can also take actions on their own initiative in order to pursue their goals.
- Social ability: Agents communicate with each other and can use their communication in order to achieve their goals.

(Epstein, 1999) adds further characteristic features of agent-based models:

- Heterogeneity: Typically, agents differ in their characteristics. For example, they may have different parameter values (e.g., age or body weight of a patient agent).
- Explicit Space / Local Interactions: Agents are often situated in a spatial environment, such as a three-dimensional Euclidean space or a network. Interactions are often restricted to the local surroundings (e.g., neighbours).
- Bounded Rationality: Agents typically do not have knowledge of everything in their environment, and their computing power is limited, for example to the use of heuristics to find an optimal decision.

An important problem is that, as (Drogoul, Vanbergue & Meurisse, 2003) note, these terms are weak and metaphorical. There is no direct translation into computational properties. The same is true for formal mathematical modelling. However, a formal description of agents should be guided by the concepts listed above.

Of all these features especially the interaction between the agents is the most remarkable. It can be found in Schelling's model as each individual communicates with its neighbours to determine whether to maintain its location or not. For a more applicable introduction to agent-based modelling the reader is referred to (Breitenecker, Bicher & Wurzer, 2014).

Properties of Agent-Based Models

The verb "emerge" can be paraphrased by "something just happens, unplanned and unintended" and is probably the best describing word for the behaviour of agent-based models. These emerging effects can especially be observed when the behaviour of some aggregated system-variables in agent-based models, depending on all agents at a time, are analysed. Electrical engineering professor Gerardo Beni (Beni and Wang 1989) was probably the first to use the word "swarm-intelligence" to describe this phenomenon, which in general (not only in models) appears when a group (respectively a swarm) of individuals shows a behaviour, which cannot (or can hardly) be deduced by the behaviour of the individuals.

It is not difficult to find reasons for the appearance of emergent phenomena in agent-based models. First of all the modeller has (or better described: "allows him or herself") no direct influence on aggregated numbers in agent-based models. Conceptualising the model the modeller needs to define the individual behaviour, target and environment of each agent, but does not define rules for the whole group, as the aggregate is already well defined by the behaviour of its parts. Hence, in order to make prognosis about the behaviour of the group it is not only necessary to know the behaviour and state of all agents, but also to know the impact of all possible combinations of all possible states of the agents on their individual behaviour, due to possible interactions between them.

Agent Based Models are a good example, how today the same modelling method approaches to be used in different domains. The two "complex" domains described in chapter one, "Complex Systems in Functional Infrastructure" as well as "Complex Decision Processes in Health Systems" both need such concepts to integrate important behaviour into the used models. Thinking on classic epidemic

(Zauner & Popper et al, 2011) Miksch et al. 2011) or evacuation-plan (Tauböck & Popper et al, 2009; Rozsenich et al. 2012) models with somewhat between five hundred and ten million agents, the resulting state space is obviously much too big to be analysed directly and can hence not be used to make prognoses about the aggregated behaviour. Steven Wolfram proved that aggregated behaviour of cellular automata can even result in chaotic behaviour (Wolfram, 2002). This result can directly be translated to agent-based models as well as their microscopic structure is usually even more complex.

On the one hand the appearance of emergent behaviour is one key motivation to perform agent-based models. In many occasions agent-based models are the only way to reproduce emergent behaviour in reality by simulation results. Hence there are a lot of possible applications for the modelling approach. On the other hand this main advantage of agent-based models is also one of the most crucial disadvantages with respect to verifiability, validity and reproducibility (see also Chapter 4.3). It can be observed that, the more complex the structure of the model, the more difficult is it to find correct parameter-sets and to determine how sensitive the aggregated model results react on parameter changes.

Agent-Based Models as Dynamical Systems

Based on the work on a project for modelling the Austrian reimbursement system and comparison of different reimbursement schemes (Einzinger, Popper et al, 2013) Patrick Einzinger defined Agents as Dynamical Systems in his thesis (Einzinger, 2014)

As „basis“ for the formalisation the discrete event system specification (DEVS) formalisms, which was originally developed by (Zeigler et al 2000) was chosen. Again as described for CAs above, some decision have to be made at the starting point. Using DEVS the approach is restricted to discrete-event agent-based systems, such that only a finite number of changes can happen in a finite time interval. The global time set should be a continuous subset of $\mathbb{R}$. Most often, it will be the finite interval $[0, t_{end}]$ for $t_{end} \in \mathbb{R}_+$.

A DEVS has an input and an output set. It can send an output from its output port to the input port of a DEVS to which it is coupled. The message passing of agents does the same, with the exception that agents do not have to obey a strict coupling. Our formal description for agent-based modelling should thus allow stochastic elements, as e.g. in health care it is usually not possible to model disease onset as a deterministic event, instead, stochastic rates are used.

To extend the classical deterministic DEVS the transition functions have to be stochastic and the concept of probability spaces is necessary. So Einzinger chose the STDEVS approach (Castro, Kofman & Wainer, 2009), that substitutes the internal and external transition function of classic DEVS with new functions $G_{int}, G_{ext}, P_{int},$ and P_{ext}. These functions generate a probability space, depending on the present state of the DEVS. Thus, a new state is not deterministically chosen, but stochastically from the probability space on the state space. We can thus define agents similar to the STDEVS:

Definition 4.2 (Agent). A tuple $A = (U, X, Y, M, G_{int}, G_{ext}, P_{int}, P_{ext}, \lambda, ta)$, is an agent, where U is the input set, X is the state space, Y is the output or message set, M is the set of modes, $G_{int}: X \rightarrow 2^X$ is a function that assigns a subset of X to every state x, $P_{int}: X \times 2^X \rightarrow [0,1]$ maps a subset of X to a probability dependent on the present state, $G_{ext}: X \times \mathbb{R}_0^+ \times U \rightarrow 2^X$ is a function that assigns a subset of X to every state x, elapsed time e since the last event, and input message u, $P_{ext}: X \times \mathbb{R}_0^+ \times U \times 2^X \rightarrow [0,1]$ maps a subset of X to a probability dependent on the present state, the elapsed time, and the input message, $\lambda: X \rightarrow Y \times M$ is the output function, and $ta: X \rightarrow \mathbb{R}_0^+$ is the time advance function.

For a given state x, the probability space for an internal transition is given by $(X, \sigma(G_{int}(x)), P_{int}(x, .))$. Similarly, the probability space for an external transition is $(X, \sigma(G_{int}(x, e, u)), P_{ext}(x, e, u, .))$.

The agents are together situated in an environment. This is the analogue to a coupled DEVS model. In this case, however, it must also be able to distribute a message to a random receiver, based on the mode of the message.

Definition 4.3 (Agent-Based Model). Agent-based model consists of agents in an environment, given by the tuple $N = (U_N, Y_N, M_N, D, \{A_d\}, G_\rho, P_\rho, \{R_d\}, \{Z_{i,d}\}, Select)$, where U_N , Y_N , and M_N are the input, output, and set of modes analogue to the agent definition, D is the set of agent references, such that for each $d \in D, A_d$ is the corresponding agent, $G_\rho: M_N \rightarrow 2^{D \cup \{N\}}$ *is* a function that assigns a subset of all agents including the environment to every mode m, $P_\rho: M_N \rightarrow 2^{D \cup \{N\}} \rightarrow [0,1]$ maps a subset of all agents including the environment to a probability dependent on the mode, $R_d: M_d \rightarrow M_N$ is the mode translation function for $d \in D$, $Z_{i,d}$ is the message translation function from i to d, where $Z_{i,d}: X_N \rightarrow X_d$ for $i = N$, $Z_{i,N}: Y_i \rightarrow Y_N$ for $d = N$, $Z_{i,d}: Y_i \rightarrow X_d$ otherwise, and $Select: 2^D \rightarrow D$ is the selection function that controls the priority for simultaneous events. For every subset of agents, it chooses one agent out of this subset.

Einzingers definition of an agent-based model is similar to a coupled DEVS model, but the output of an agent Ad is not simply passed to connected agents. Instead, the output message has a mode m with it, which is translated by the mode translation function Rd to a mode $m' \in MN$ of the environment. According to this mode, the functions $G\rho$ and $P\rho$ construct a probability space on the set of all agents including the environment itself. This models that the message can go to any other agent or to the output of the environment.

I remarked at the beginning of this section that, by choosing DEVS we are restricted to discrete-event agent-based systems. After summarizing the steps for a formal agent based concept, which we can now use in future for comparison and coupling, a next step will be to formalize the concept with Zeiglers DEVS/DES approach, which we already used to model manufacturing systems (see chapter 4.6) Fort he connection to stochastic dynamical systems I refer to (Einzinger, 2014)

Analytical Methods to Analyse Agent-Based Models

As sensitivity analysis is an indispensable part of validating any model, it is necessary to perform some deeper model analysis for agent-based models too in order to produce a reliable model. Compared to e.g. differential equation models, for which a sensitivity analysis can be performed by calculating a simple Jacobean, this task is a lot more difficult here. In most cases a classic parameter-sweep is the only way to get the reactions of the group on individual parameter changes. As agent-based modelling is already a very time and memory consuming modelling technique a parameter sweep is an extremely expensive procedure here.

Hence it is a very famous task to derive analytical methods to approximate the aggregated behaviour of such kind of models by some state-space reduction method. In general most of these methods try to reduce the state space so that it becomes independent of the number of agents using some version of the law of big numbers.

One example for this process is the so called diffusion approximation (van Kampen, N. G., 1982). Hereby the behaviour of the empiric mean of all agents is approximated using a set of ordinary differential equations which can be parameterised with the individual rules of the agents. In general Markov-theory poses the base for a big class of similar investigations, usually called mean-field analyses. In most cases correlated theorems end up with difference equations (Gast and Gaujal 2011), ordinary- (Boudec, McDonald, and Mundinger 2007) or partial-differential equations (Deffuant et al. 2000) which can be directly be determined based on the parameters of the agent-based approach. As theory about stochastic processes is usually very tricky and restrictive the involved mean-field theorems unfortunately have a very limited field of application:

- Although all those approaches tend to reduce the state space by elimination of the number of agents, increasing complexity of the interaction between the agents leads to a blow-up effect for the state space of the resulting differential (difference) equations.

- The agent-based model basically needs to be memory-less (somehow Markovian) – that means each agent decides based on its and its contact partners current state. If a memory (like e.g. in form of a learning process) is involved, almost every workaround leads to a blow-up effect for the state space of the equations as well.

- Complex spatial behaviour of agents like very specific movement rules on complex geometries or networks can hardly be approximated.

- Almost every type of state transition in the agent-based model somehow needs to be resolved to happen with some probability or rate. Very often these probabilities need to be estimated and approximated which is a big source of errors.

Hence there are lots of very simple examples for which related theorems lead to reliable approximations (see at the example of the SIR (susceptible-infected-recovered) epidemics model in (Bicher & Popper 2013), but unfortunately the mean-field theory is hardly ready to support realistic applications usually involving very complex individual behaviour. Hence there are still many unanswered research questions.

As the characteristics of certain modelling approaches are not suitable for mathematical analysis it is sometimes useful to re-design (parts of or a simplified version of) the conceptional-model with a different modelling technique. Hereby it is necessary to first of all determine a level, where both modelling approaches can be compared, and second of all analytically verify that both modelling techniques lead to the same results.

An example for this idea is given in (Bicher 2013), comparing microscopic and macroscopic modelling approaches. It is shown that for certain simplified, stochastic agent-based models systems of usually highly non-linear ordinary differential equations describe the temporal behaviour of the expectancy value of the aggregated number – often called the mean field:

$$\phi_d(t) := E\left(\frac{1}{N}\sum_{i=1}^{N}\chi_d\left(a_i(t)\right)\right).$$

Using this aggregated level is a commonly used standard for the aggregated analysis of microscopic modelling approaches as it counts the fraction of agents a_i sharing state d at time t. For a discrete state space the following formula can be derived based on the diffusion approximation for Markov processes (see (Kampen, N. G. van 1982) describing the temporal behaviour of this aggregated number:

$$\phi_d' = \sum_{k \neq d} \phi_k W_{kd} - \phi_d W_{dk}, \qquad \phi_d(0) = \frac{1}{N}\sum_{i=1}^{N} \chi_d\left(a_i(0)\right).$$

Hereby W_{kd} denotes the probability that a random agent in state k changes to d in one time-step. For a derivation and application of this formula we refer to (Bicher 2013). Again a directly applied derivation of the theorem is found on the example of the famous SIR differential equations (Kermack & McKendrick, 1926) in (Bicher & Popper 2013) proving the equivalence of different modelling methods applied on epidemics.

Hence at least the aggregated number of an agent-based model, which is usually difficult to analyse mathematically, can be compared with a corresponding system of differential equations which mathematical background is very well known.

Summary

Both, for the formal definition presented but also for all analytic methods based on it still there is the problem that the number of agents has to be constant, i.e. it is not possible for agents to be created or destroyed. We have taken some steps in formalising the concepts and preparing the models for a mathematical analysis. Still this is an important lack to model complex system, as creation and destroying of sub models or agents is an important characteristic of complex system. Based on this example we can see the trade-off very well. Classical methods for defining cellular automatons or agent based models can easily include creation and destroying of elements, or can easily integrate other characteristics like stochastic processes. Introducing formal definitions to improve mathematical possibilities force us on the other hand to restrict the features for the sake of analytic description. One main aspect of this work is to show examples like above, to outline how to develop a „stepwise“ strategy, where the given approaches and examples should converge for improving the capabilities of "comparative modelling". In the next section I will give a short outline about coupling methods. As long as we cannot develop models which map different systems to one model effectively, there results a need for coupling of computational models.

3.3 Coupling of Methods

As described in chapter 1.1 one application for complex system simulation are large infrastructures with heterogeneous processes. An application is the area of airport planning. The planning of airports has been getting more important in the last years, since the amount of passengers being transferred increases constantly and a deeper understanding of results calculated by simulation experiments is necessary. Also the restrictions in planning according various ecologic effects are getting more restrictive as well. By optimizing buildings and especially large buildings in the early stages of planning savings of material and money can be achieved. If space is seen as an endless resource diverse ways of looking at a problem arise. If too many resources were planned the utilization of these resources can be seen as less efficient over time, which leads to unnecessary built space that needs expensive maintenance and inefficiency in the business. Some examples are: increased expenditure of energy or other resources, rising impervious surfaces. Inefficient process on built space can be made visible only by the dynamic utilization of space. With new strategies and intellectual approaches it will be possible to see space, its functionalities and its processes as ecologic relevant resources. The overall aim of modelling and simulation is to reduce the economic expenditures, as well as in increase the positive ecologic aspects. Also accessibility and transit time lengths are in the airport planning and other application areas very important components of the simulation. Usual planning errors like to small turning radius in toilets for wheel chair drives and inacceptable access paths for handicapped persons can be avoided. Different stakeholders need to be satisfied as well. For example projects in the area of airport planning on the development of air infrastructure address not only the planners and airports, but also the effects on industrial and touristic development of the whole region. These different views of planners, architects, airports, ministry, passengers and people who live in that region need to be included in a simulation and the interpretation of the results. This is an example why trade-offs in simulation of large infrastructure developments are not welcome and why a different approach is needed.

The systems that need to be modelled are getting more and more complex and interconnected and that is why modelling a single subsystem is not enough anymore. Complex behaviour arises through the interconnection of the different subsystems. For example: The Airport City consists of a large set on subsystems, like the landside, terminals and airside as seen in 3.2 and many more.

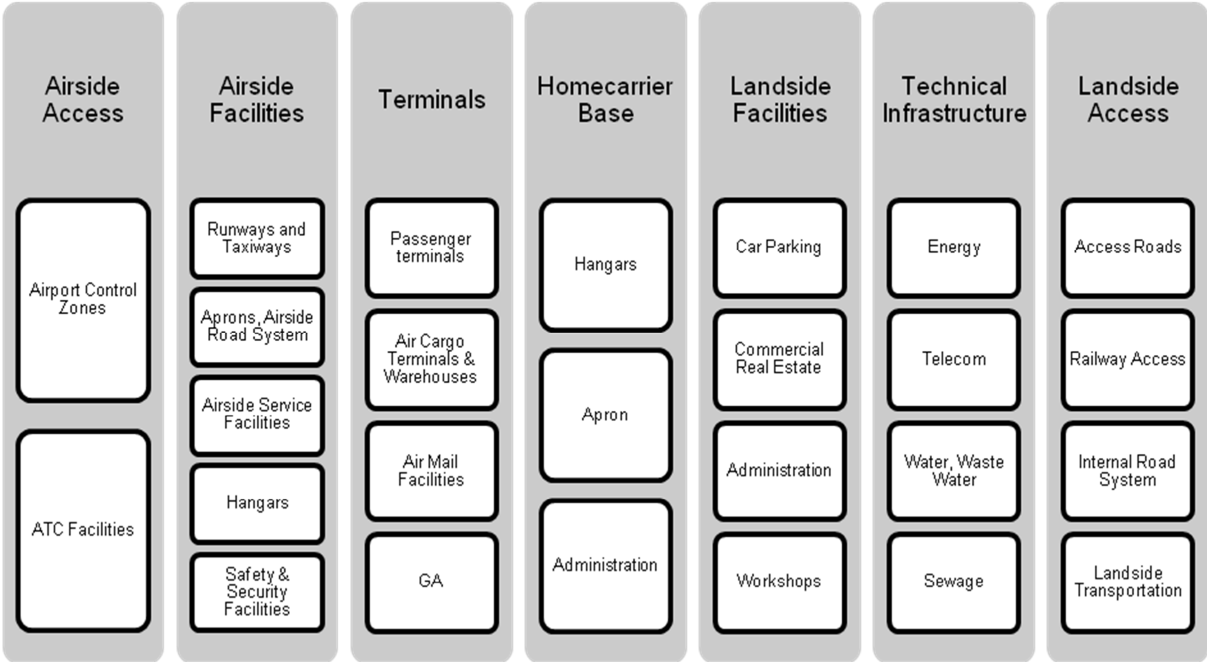


Figure 3.2: Subsystems of the Airport City

Passengers arrive by plane (on the airside) and by car, bus, train or taxi (on the landside), then proceed to the terminal and retail area, utilize resources, and also consume resources and spend resources (retail area, technical infrastructure for water and sewage). Personnel are required and have to be planned optimal to avoid over- and underutilization, but all to the end that a quality standard is improved or at least stays above a level, good working conditions are reached and that there is still a profit for the different stakeholders together with ecological thresholds being strictly adhered. These different aims addressed at a simulation model seem to be contradicting.

3.3.1 System Assessment

If the research question addresses the utilization of resources in the terminal system, also the question of how people even arrive through airside (passengers coming by plane) or landside (passengers who want to fly away and arrive by car, bus, etc. on the landside) have to be answered. So for the sake of an example, why the coupling of d subsystems modelled with different modelling methods is necessary, two models modelling the Landside and the Terminal Area of an airport are described.

The Landside is the part of the airport in front of the airport building, as seen yellow in Figure 3.3. Different processes are going on there:

- Passengers who want to fly away arrive by car (drop off or parking), bus, taxi, limousine or train.

- Passengers who arrive by plane and want to proceed to the city or somewhere else.
- Personnel arrive to go to work.

Figure 3.3: Overview of the Vienna International Airport where different zones are marked in different colours. Landside is the area where cars and so on arrive and terminal area is where passengers check in and go through controls.

The research question is if the available resources are over or underutilized and what happens if a road or a parking area is closed due to construction or emergency, especially what effect it has on the traffic development.

In this case an agent based model suits best: Agents are cars and they follow specific rules (priority, drive on street, let pedestrians cross on crosswalks, park only in allowed areas, etc.). The environment is the floorplan and last but not least agents can have different behaviours like “drive angry” or “drive carefully”. This means that there are different behaviours associated with the agents and in this simulation individual behaviour is necessary to model since real time traffic simulation is required. There is a road net that has to be followed, but a car can choose where to go. So all features described in section 3.2 are needed and can be modelled as well.

The terminal is the part of the airport, as seen pink in Figure 3.3, where passengers check-in, drop off luggage, go through security checks and passport controls. Here the passenger doesn’t need to have an own behaviour, because the processes going on there are strictly predefined. The research question here is also addressing the resource utilization as in the previous model, but with additionally calculation waiting time for passengers (which is a quality measure indicator). The passenger is now called an entity and is being passed on working off his goals through the terminal. The goals are defined by servers that require resources (personnel) to work off the passenger. In this case a model that doesn't need so much calculation time as the agent based model, and where passengers don't have an individual behaviour or can choose by themselves where to go is required: a discrete event model suits this case perfect, where the major changes in the states of the system only happen at discrete time points.

Now one can build the model on its own, not taking into account the results of the landside simulation. But, what happens if there are delays on the landside and passengers cannot arrive on time at the terminal and furthermore arrive after the delay is removed all at once? So, building the terminal model on its own is not enough and requires the input from the landside model. The connections of those two models are on the one side through the passengers and also the personnel that arrive through the landside to go to work in the terminal (and other areas and also leave that way).

Furthermore, connections from the airside to the terminal and then to the landside have to be modelled as well, since passengers also arrive by plane and go the other way round. In this specific example the agent based model (with cars being agents) and the discrete events model (with passengers being entities) are connected through a specific defined interface. Coupling a discrete event model with an agent based model can be established by every time an entity enters the sink an agent in the agent based model is generated and vice versa. In this case for each car a setting of number of passengers was originally calculated in the agent based model, because data in form of number of passengers was available. When cars find a parking lot, the passengers proceed to the terminal model and in the discrete event model the number of passengers is generated. In this case also the usual problem with continuous and discrete time is no problem, since the discrete event model is modelled in continuous time, only the changes of the state happen in discrete time. Events responsible for those changes don't have to be in equidistant time, but can also be in dynamically calculated time spans. The only condition is that in between two following events nothing else happens and this is guaranteed.

The data that is used in this simulation is taken from the design peak day that specifically provided for simulation by the Vienna International Airport and includes data on in- and outgoing flights with registered destinations and number of passengers amongst other variables. The data for one day together with planned and actual timestamps for leaving respectively arriving planes is given.

Not only micro based simulation methods can be applied and used for multi-method (or modular) modelling, but also macro simulation methods like System

Dynamics, when it comes to questions addressing the economic outcome of a subsystem.

3.3.2 Hybrid Simulation

Researching literature done by Barbara Glock and the author (publication at I3M 2015) showed that there are multiple terminologies for modelling a large system with different modelling methods. Searching databases like ScienceDirect, Scopus, Springer Link, IEEE Xplore and MathSciNet by using terms and their combinations like "hybrid modelling" and "coupled models" in the first place, showed that other terminologies like "dynamic system modelling", "hyper modelling", "interconnected simulation", "interfaced simulation", "integrative modelling", "multi-method modelling" and many more are used for this kind of modelling as well. (Swinerd & McNaught, 2012), (Sargent, 1994) and (Lättila, 2010) refer to it as "hybrid models" or "hybrid modelling". They also proposed some methods of coupling Agent-based and System Dynamics models. (Scholl, 2001) referred to this kind of modelling as "multimethod and integrative approaches" and (Schieritz, 2003) referred to it as "integration", which makes it intuitively clearer what is meant than just saying "hybrid" modelling. (Fishwick, 2012) extends the meaning of "integrative modelling" or "multimodelling" and introduces a new term "hypermodel" to include interaction within models, among models and between human and models. On the other hand some of these terms, like "hybrid" are used for more specific or other interactions, like it is done in Discrete-Event Modelling and Control of Hybrid Systems by (Nixdorf, 2002): "hybrid" has a different definition in the context of modelling and simulation here and means that within one model discrete and continuous elements are modelled. Basically said, there are a lot of terms used for what intuitively might be best understood as multi-method or modular modelling.

Before we go on proposing what a modular model in our context is, we need to recapitulate some definitions first. A system is a collection of interacting or interdependent objects. The objects are the components of the system. (Definition 1.4) A subsystem is a set of elements, which is a system itself, and a component of a larger system. The system can be decomposed into subsystems where each of them can be modelled with another modelling method, forming a sub model.

The sub models for these parts of the system can be parallel or sequential and they can be on the same level or ordered hierarchically.

Definition 4.4 (Modular Model). A Modular Model is a model that consists of at least two sub models, where at least two different modelling techniques are used.

These sub models exchange information in some way. This process of information exchange is called coupling.

As described in section 3.3.1 two examples in the domain of airport planning were presented. After the definitions above both modelling methods described above can be used for implementation of a modular model. In addition (as mentioned above) System Dynamics is also widely used in this domain.

Agent-based modelling and Discrete Events are micro-based or individual-based modelling methodologies, best suited for modelling systems where the behaviour of (autonomous) individuals determines the behaviour as described above, see also (Bonabeau, 2002; Macal & North, 2010). Discrete Events models are similar, but the entity modelled here is not like an agent autonomous, but is passively led through the system instead. Furthermore, changes in the state of the system happen due to events at discrete points in time (Zeigler, 2000). In between two consecutive events the state remains unchanged. This kind of modelling is mostly used in logistics and transportation. Another paradigm is set by System Dynamics modelling. Here the point of view is from another level, where only aggregated levels are looked at. It was developed in the 1950s by Jay W. Forrester, who applied it first in management systems (see Industrial Dynamics (Forrester, 1997) or Urban Dynamics by Forrester (Forrester, 1973)). He then transferred this methodology to social systems. Nowadays diverse literature on System Dynamics and Systems Thinking exists (Sterman, 2000). A SD model consists of stocks and flows, which basically is a set of differential equations. The dynamics of the system emerges from causal links of the modelled variables that often form feedback loops. Application areas are economics, health care, policy design.

3.3.3 Definition of Coupling

Researching now the effects that emerge by interconnecting these subsystems, this calls for a coupling of the different modelling methods, as mentioned before. So all advantages of these methods used for modelling the larger system can be integrated. Sargent (1994) suggested, based on his definition of a "hybrid model", which "is a mathematical model which combines identifiably simulation and analytic models", four classes of hybrid models (see below) According to (Swinerd & McNaught, 2012) there are four classes of hybrid models that combine analytical models and simulation models. They used that concept for these kinds of models, because most of the time these two model types are used: Analytical models are cheaper to build and simulation models are more realistic. They then transferred that concept into one for Agent Based Models and System Dynamics models, but the definitions for these classes can be more or less transferred to all kinds of different modelling methods. The four classes, as presented in Figure 3.4. are:

1. Class I – "a model whose behaviour over time is obtained by alternating between independent analytic and simulations models".
2. Class II – "a model in which an analytic and simulation model operate in parallel over time and with interactions between them".
3. Class III – "a model in which a simulation model operates in a subroutine way for an analytic model of the total system".
4. Class IV – "a model in which a simulation model is used to model the total system but which requires values for a portion of the system or input parameters, from an analytic model".

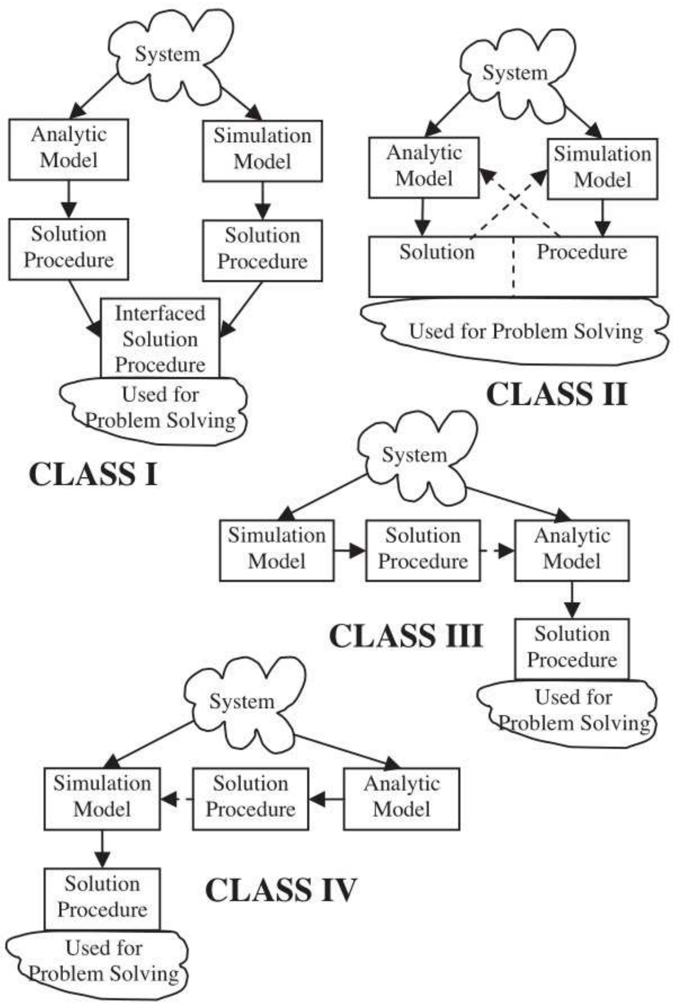


Figure 3.4: Different classes of hybrid modells according to (Swinerd & McNaught, 2012)

Sargent (1994) already found out that, what we call modular or multi-method modelling, is needed to be researched, because these kinds of models are very useful in different application areas and have a lot of potential in modelling the world in a more realistic and effective way.

Barbara Glock focusses in her recent work on the application of this concept on Agent Based models and System Dynamics, for details see Glock et al, "Various Aspects of multi-method modelling and its applications in modelling large infrastructure systems like airports", submitted for I3M 2015 conference). We want just shortly present the concept, which can be used for all modelling concepts.

Swinerd and McNaught (2012) derive three classifications (Figure 3.5)

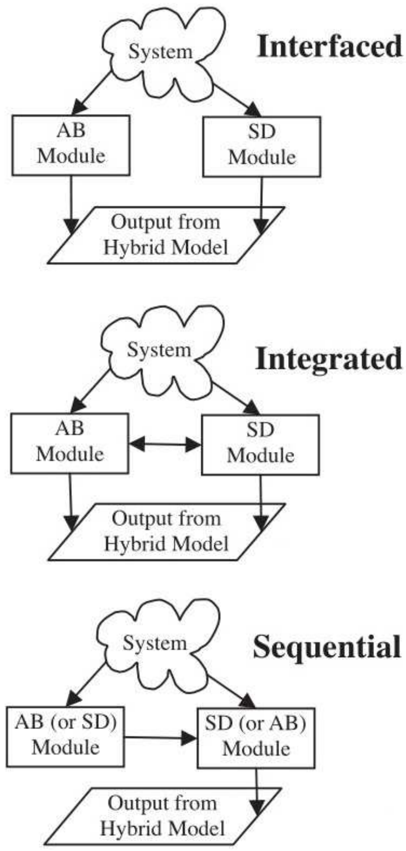


Figure 3.5: A Classification of Multi-Method Models according to Swinerd and McNaught (2012) for modelling Large Systems

Definition 4.5 (Interfaced Model). An interfaced model consists of two sub models with different modelling methods and have some point of interaction or communication between elements; the sub model run alternating and independently.

An Interfaced model is equivalent to Class I above. An example for an interfaced model as given in Swinerd and McNaught (2012) is: an AB sub model where a person (agent) walks along a street trying to reach his goal. Public traffic transportation is modelled by another sub model in DES. The agent can decide (within the AB sub model) if he wants to walk (stay in AB sub model) or if he wants to take the bus (DES sub model). He is either in one sub model or in the other, hence independent sub models that run alternating. Andreas Körner is dealing with such interfaced models for another domain, where DAEs are used in his PhD thesis (Körner, 2015). As a matter of fact it is an important approach to match these different work on different domain and to maintain a common formalisation.

Definition 4.6 (Sequential Model). A sequential model is a model consisting of sub models, where one sub model needs the output from the other sub model as input.

Sequential Models are equivalent to Class III and IV described above.

Definition 4.7 (Integrated Model). An integrated model is a model, where different sub models operate in parallel over time and with interactions between them.

Integrated Models are equivalent to Class II above. An example for an integrated model of agents with rich internal structure is an AB model where each agent contains a SD model, as the agent's "brain" or a model with stocked agents, where it is "a level within an SD model that is used to bound an aggregate measure of an AB module" (Swinerd & McNaught, 2012).

Basically, there is a fine line between the classes of modular models and the modeller has to decide what fits best. It is also dependent where the system boundaries lie.

Application in Airport Planning

Landside and Terminal Subsystems of an airport were described above in the section 3.3.1 "System Assessment". In this section I only outline the concept for coupling; of course this modular setup can be extended for other subsystems and other applications.

Research questions developed are if resources like personnel and number of open counters in the terminal are sufficient at each time to maintain the quality standards measured in waiting time of passengers. This being a simple server-queue question is modelled best using Discrete Events with counters and personnel being resources and passengers being entities. For the landside the research question is if the available resources are over or underutilized and what happens if a road or a parking area is closed due to construction or emergency, especially what effect it has on the traffic development. We could no try to develop one model for both subsystems.

Following the approach of chapter 3.2 we could model the discrete event model using Zeigler's DEVs formalism and an Agent Based Model also with STDEVS. But as shown in chapter 3.2.2 the effort for the model would increase without benefit for the model.

So in the given case we use the additional possibilities to define an integrated model with a discrete event sub model and an agent based sub model. We can now model all defined characteristics from chapter 3.3.1 sufficiently. Details for implementation are shown by Glock in her actual work (see submitted publication above).

The aspect of importance for the theoretical concept is that the approach can iteratively be applied to the system: Even within the Terminal, we probably need two sub models, one discrete model for the queuing process and one agent based model for behaviour of passengers e.g. for shopping. The retail area is economically seen a very important part of the airport since a large part of the profit is gained by the retail area. The retail area is a shopping area after having passed the controls in the terminal where passengers go through when they proceed to the gate to depart. One main research question in this area would be to maximize profit by guaranteeing a specific level of quality standard for passengers like a short way to the gate or attractive sales. But for these questions the passengers would be better modelled as agents and not as entities of a discrete model. So we could use an AB sub model that includes spatial information (map of the shops) where passengers walk through the retail area as agents. The environment is the retail area with the shops. Depending on specific features of the passenger, like if he is business or tourist (only hand luggage or not), or what his destination is (if within Schengen, then the passenger can proceed without passport control) additional sub models can be developed. This sub model could also include transfer passengers, meaning passengers arriving at the airport by plane, going through passport control if necessary and proceeding to gate after going through retail area. This circumstance would need additional features.

It also shows, that this sub model might need input from the landside as well as from the airside and if some delays or other effects happen in the parts of the airport not represented in the terminal sub model it has an effect on the terminal sub model. So we habe to extend the model to the Airside area (Magenta Planes in Figure 3.3).

By using different (best fitting) modelling methods for different subsystems and utilizing all their advantages on the one hand a more realistic presentation of the modular model can be created (what makes communication to decision makers easier) and on the other hand accumulating errors can be eliminated to some extent.

3.3.4 Co-Simulation

In section 3.3. we did not focus on the questions of implementation of the resulting computational models. Besides the modelling tasks, e.g. how to deal with the runtime coupling of aggregated and individual based models (agents) or dealing with state events (see Körner, 2015) of course computational problems arise and are a main challenge to cope with. In this work I can only mention some aspects, e.g. the approach of how to coordinate the computation of different models implemented in different simulation tools. *„Nowadays it has become more and more important to be able to simulate models with partial models of different complexity and differing requirements regarding solver algorithms, step sizes and other model-specific properties. To meet these requirements, models of such complexity are approached via co-simulation."* (Hafner et al, 2012a)

As described co-Simulation is a good example how such problems are treated at the moment, as parallel simulation of models using different simulators is coordinated with one overall simulator. The idea is to match all needed features for the model with different (existing and well tested simulators) (see also Hafner et al, 2012b). Depending on the interdependencies between the partial systems, we can distinguish between loosely coupled systems and strongly coupled systems. For further inspections, let

$$System\ 1: \dot{y}_2 = f_1(y_1, y_2, t), y_1(t_0) = y_{1,0}$$
$$System\ 2: \dot{y}_2 = f_2(y_1, y_2, t), y_2(t_0) = y_{2,0}$$

The two systems are called loosely coupled if $\left\|\frac{\partial f_1}{\partial y_2}\right\| \ll \left\|\frac{\partial f_1}{\partial y_1}\right\|$ and $\left\|\frac{\partial f_2}{\partial y_1}\right\| \ll \left\|\frac{\partial f_2}{\partial y_2}\right\|$, i.e. the variables needed from the respective other system have a rather small influence on the regarded system in comparison with the variables calculated by the current system itself (see Striebel, 2006).

In this case, multirate simulation can be considered. Multirate simulation allows each participating system to use its own time step (or even solver and simulator, if desired), synchronize at certain steps in time given by an overall solver and use extrapolated or interpolated values for the ones needed from the other systems. Applying multirate simulation is sensible if the time constants of at least two participating systems differ gravely so the slower system would have to unnecessarily calculate states at all points in time the faster system requires for accuracy. An example for a system divided into two parts with hugely differing time constants would be a production hall consisting of the thermal model of a building and one or more machine models with mechanical, electrical and thermal parts. The systems have to be linked according to Figure 3.6 since the building needs to know the machine's heat emission to calculate the room temperature.

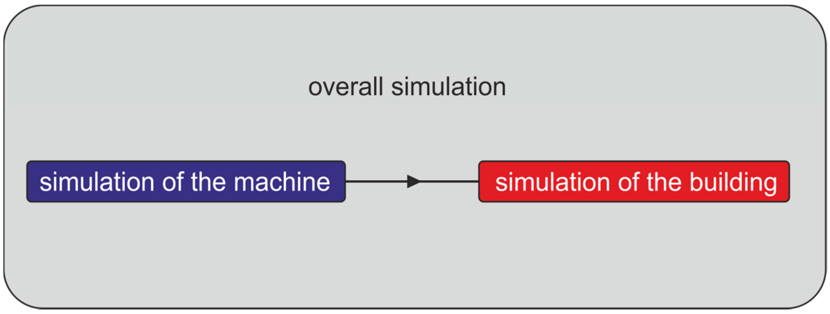


Figure 3.6: Sequential Model of a production hall

The thermal processes in the building are reacting rather slowly and probably will not need to be calculated more often than every few minutes whereas the electrical processes in a machine require time steps of fractions of a second. It can be clearly seen that it would be unnecessary for the simulation of the building to take the same, small steps as the simulation of the machine. Instead, by applying a multirate method it is possible to let the machine be simulated with its own, small time steps while the simulator for the building takes larger steps which in addition correspond to the time step for synchronization. These steps do of course have to be part of the time steps for the simulation of the machine, too, to enable synchronization. Figure 3.7 shows the steps taken by the individual simulators of the system described above.

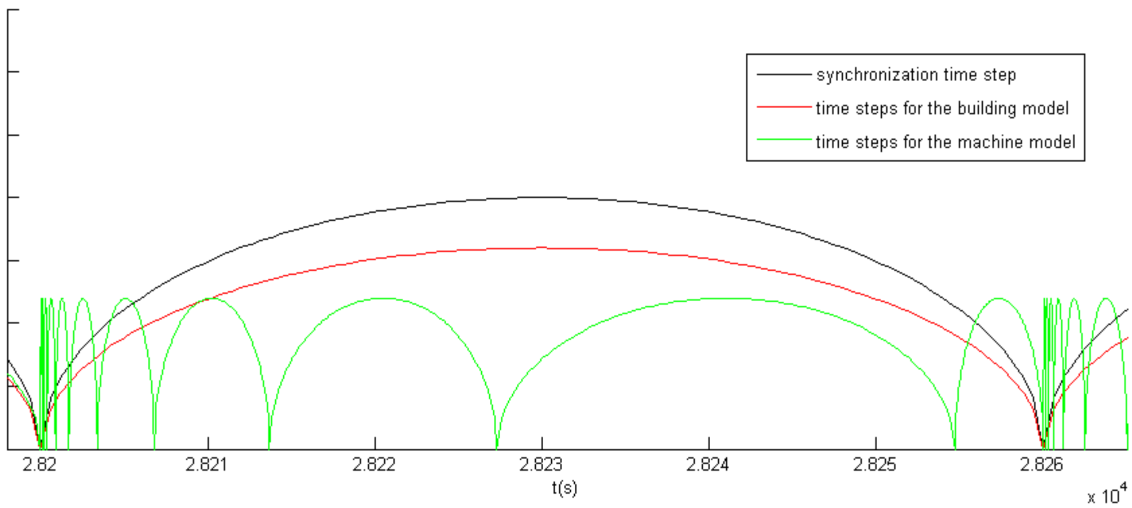


Figure 3.7: Multirate Method

Most applications requiring co-simulation do not only consist of two systems with connections only in one direction. Figure 3.8 shows the intended communication of the simulation of a production hall including four partial systems: a model of the building, two machines and a control model for the regulation of the room temperature.

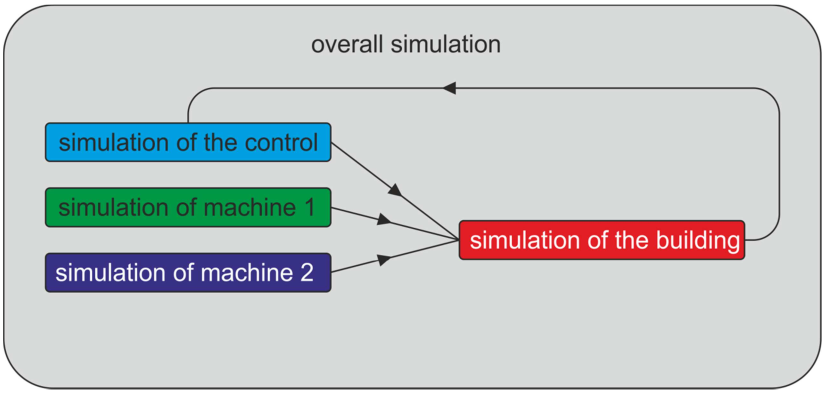


Figure 3.8: Integrated Model of a production hall

The crucial part of multirate co-simulation is the approximation of accuracy loss resulting from the extrapolation in between synchronization references.

If high accuracy is required but co-simulation is necessary not due to highly differing time constants but different modelling approaches and requirements regarding the implementation, strong coupling will be considered. With this kind of co-simulation, the time step is chosen globally and iterations between the simulators take place in each time step to assure a given accuracy of both the individual systems as well as the overall system, see (Trčka, 2008; Busch, 2012) for further information.

In this section we could get a short glance how the described modular modelling approaches (section 3.3) directly influence the concepts of implementation of the computational models. Depending of the type of modular model (sequential, integrated, interfaced) in future different solvers and controllers for hybrid simulations will be needed.

3.4 Introducing Interventions in Health System Research

We have seen now development of model comparison and coupling, as well as resulting problems. Another concept is the idea of transferring "off line" modelling concepts between domains. As a matter of fact here we don't have the problem of formal comparison or run time coupling. But we have to find out if the modelling concepts can be applied to the domain immanent structures. Again we focus on an example for outlining the most important aspects.

Based on the example of Chapter 2.2 we assume, that our SIR Epidemic want to be treated by interventions. Our general model can integrate such interventions as follows. In order to confine an epidemic, interventions might be applied. We define two different types of strategies ("soft" and "hard") that can be applied when a certain critical threshold of infected individuals is reached or exceeded. The threshold is defined relative to the whole population as $f_T N$.

As a "soft" strategy, the system parameters C, α or β are decreased to $f_S \cdot C$ (or $f_S \cdot \alpha$ or $f_S \cdot \beta$) over a period of time Δt. $0 \le f_S \le 1$ is called the reduction parameter. This can be either a linear decrease in the form $f(x) = k \cdot x$ or a smooth step in the form $f(x) = 3 \cdot x^2 - 2 \cdot x^3$. Let $r(t)$ be the function that describes the decrease from 1 to f_S, so that it can be multiplied with C, α or β, and let t_T be the time when the threshold is reached. For a linear decrease

$$r(t) = \left(1 - \frac{t - t_T}{\Delta t}\right) + f_s \frac{t - t_T}{\Delta t} \qquad 3.1$$

and for a smooth step it can be

$$r(t) = 1 - \left(3\left(\frac{t - t_T}{\Delta t}\right)^2 - 2\left(\frac{t - t_T}{\Delta t}\right)^3\right) \cdot (1 - f_s). \qquad 3.2$$

If $\Delta t = 0$, then the change is a discontinuous step. Figure 3.9 illustrates the idea and expected outcome of a "soft" strategy. Once the number of infected reaches a critical threshold, the infection parameter decreases over a certain period of time.

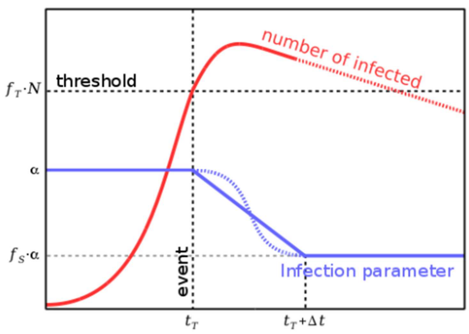


Figure 3.9: Illustration of a "soft" intervention in a SIR Modell.

"Hard" strategies involve the individuals directly. Representing a quarantine or vaccination strategy, susceptible or infected individuals, respectively, can become recovered. Such a "hard" strategy is defined by choosing a fraction f_H of susceptible or infected individuals and immediately changing their state to "recovered" when the threshold of infected individuals is reached. The individuals are chosen randomly among all possible individuals with the respective state, since further distinction is not possible with this system definition. Table 3.1 lists all parameters that are relevant for interventions.

It could be that the threshold is reached more than once. This happens, for example, when the number of infected is growing, then it is reduced by an intervention but still keeps growing. The intervention strategy can be applied in two ways: either only once when the threshold is reached for the first time or every time it is reached.

Parameter	Description
$\boldsymbol{f_T}$	Fraction that defines the threshold
$\boldsymbol{f_S}$	Reduction parameter of a soft intervention
$\boldsymbol{\Delta t}$	Duration of a soft intervention
$\boldsymbol{f_H}$	Fraction parameter of a hard intervention

Table 3.1. Parameter of hard and soft interventions.

For the two models these concept results in easy to adopt model interventions. For the ODE system we get for a "soft" intervention strategy, the parameter γ or δ in the ODE system needs to switch to a time dependent function $\hat{\gamma}(t)$ or $\hat{\delta}(t)$ when the threshold $f_T N$ is reached at time $t = t_T$.

$\hat{\gamma}(t)$ or $\hat{\delta}(t)$ calculates as the term in Table 3 where the desired parameter C, α or β is replaced by $C \cdot r(t)$ or $\alpha \cdot r(t)$ or $\beta \cdot r(t)$, and $r(t)$ corresponds to the function in Equation for linear decrease or smooth step.

At time $t = t_T + \Delta t$, the ODE system switches back where γ or δ is replaced by $f_S \gamma$ or $f_S \delta$.

In a "hard" intervention strategy the ODE system abruptly changes $S(t)$ or $I(t)$ when the threshold is reached. This can be achieved using the delta distribution $D(x)$ where $D(0) = 1$ and $D(x) = 0$ for $x \neq 0$

For example, quarantining the fraction f_H of infeceted individuals when the threshold is reached, then the ODE can be rewritten as:

$$\begin{aligned} S'(t) &= -\gamma \cdot S(t) \cdot I(t) \\ I'(t) &= \gamma \cdot S(t) \cdot I(t) \\ &\quad -\delta \cdot I(t) - D(I - I_T) \cdot f_H \cdot I(t) \\ R'(t) &= \delta \cdot I(t) + D(I - I_T) \cdot I_Q \end{aligned} \qquad 3.3$$

For the LGCA model we get for interventions Also for the CA approach intervention scenarios can be simulated. If the number of infected particles in the CA reaches the threshold, one of the strategies described can be applied.

Applying a "soft" strategy is easy for α and β. Then, φ or ϕ are multiplied with $r(t)$ so that the $f_S\varphi$ or $f_S\phi$ are reached after Δt. Reducing C causes problems because it requires a change of n. First, changing n is very inaccurate and second, there is no instruction on how to enlarge or shrink the space in respect to the individuals that have positions on the grid. Thus, if a "soft" strategy for C is desired, it should be performed very carefully.

"Hard" intervention strategies can be directly applied as stated in the system definition. Then the threshold is reached, a desired number of susceptible or infected individuals are randomly chosen, and immediately become recovered.

In contrast to the ODE model, individuals in the CA are distinguished by their spatial location on the lattice. Presumably, the selection of particular individuals/particles for changing their state can make a crucial difference. For testing purposes, it seems reasonable to deliberately violate the system definition and choose individuals with respect to their location.

As both approaches are well defined, still the application to a real world application is not satisfying. Real interventions could not be modelled with these approaches. But what would be, if there are methods validated in one domain, which might be useful for example to introduce interventions in the health system. One would have to evaluate the classical methods used in one domain and analyses the question, whether or not the method would be applicable and sufficient to be used in another domain. An example for such a process will be shown in section 3.4.1.

3.4.1 Discussion of the Problem

In order to model problems in the health care system, especially for the economic evaluation of medical technologies, different methods of model design are used. Today patient centred approaches get into the focus of activities more and more. So models need to implement patients reality and needs as system requirements. Furthermore it was and still is not possible to analyse interventions limited to specific groups of patients and measures that impact divers groups of the population differently in a suitable manner.

A well established method and simple method are the so-called Markov-Models. Here the distribution of a cohort of persons on different (health) states are calculated for every discrete time-step (Siebert et al. 2012). Though, in this method all interactions between individuals are prohibited, which would be necessary for simulating epidemics.

Therefore, other methods are required. The modelling through ordinary differential equations (ODEs) and the equivalent method System Dynamics are equation based approaches (Brailsford 2008). The consideration of interactions is therefore possible. Furthermore it is the predominant method for models, where a dynamic spreading of diseases takes part (Pitman et al. 2012). Also heterogeneous populations (differentiated in gender, age and socio-economic status, for example) can be mapped through the according separation in the state space of the equations. Nevertheless, interventions still present a challenge using this method.

If ordinary differential equations are combined with algebraic ones, so called constraints, they result in differential-algebraic equation systems (DAEs). These are mainly used in mechanics and electrical engineering. Here they appear for example in the derivation of equations of motion by using the Lagrangian formulation. Variational problems with holonomic auxiliary conditions generally lead to differential-algebraic equation systems (Giaquinta 1996). Describing the model through the Modelica-standard also leads to differential-algebraic equation systems, which have to be suitably simplified and solved through the solver. Furthermore, physical and chemical processes are often described through differential equations, while also algebraic equations may appear through different laws, like Kirchhoff's laws or conservational laws (Weiß, Daniel 2007).

Outside of the technical-area differential-algebraic equations can appear too, for example when extending differential equation models through constraints. This is described, for example, by T. K. Kar and Kunal Chakraborty, who have derived a differential-algebraic equation system froma predator-prey-model, a normal differential equation, by introducing an economic factor (Kar and Chakraborty 2010).

Applications of such methods in the health care system are rarely found in the literature. For example, classic epidemic models like SIR or SEIR might be described as differential-algebraic equation systems (Yi et al. 2009). However, these systems just have Index 1 and can therefore be treated easily.

Realistic constraints and their effects on different population groups, for example the specification of a limited and fixed budget, which has to be distributed, cannot be dealt with up to now, because they might lead to differential-algebraic equation systems with a higher index. These conditions are generally of importance when treating optimal calculation of resources, when there is a total amount of money that has to be distributed to various interventions for different groups of patients, while maximizing the desired effects. Hereby the "maximum" has to be defined properly when specifying the research question. Up to now such problems are mapped through ordinary differential equations or other modelling methods that do not include constraints and the distribution of the budget is calculated through the application of suitable optimization methods. The fixed budget is thereby defined as an auxiliary condition for the optimization.

These problems of optimization concerning the calculation of resources in health care were, among other things, analysed for interventions controlling epidemics (Kasaie and Kelton 2013; Lasry, Zaric, and Carter 2007; Sharifi 2014). Moreover, the optimal distribution of means of prevention, treatment and research of cardiovascular disorders are studied by Miller, Daly and Roehrig (2013).

The studies described here have in common, that the distribution of resources is fixed externally as parametrization for every simulation run. Up to now problems, where the distribution cannot be defined directly, but indirectly, coming out of the state variables of the model (e.g. the amount of patients with a specific treatment) were not considered. Thereby the actual variables have to be arranged in a manner to comply with the fixed budget.

Besides Markov-Models and differential equations also other approaches for the modelling of problems in health care are used. Especially individual-based (microscopic) methods are of interest, for example agent-based models (Macal and North 2009), cellular automata (Schneckenreither, Popper & Breitenecker 2008) and micro-simulation-models (Rutter, Zaslavsky, and Feuer 2010). These approaches are especially popular in the areas of health care economy, demography and epidemiology (Jaffry and Treur 2008; Spielauer, Martin 2007). These models are more flexible than equation-based models, because interventions of the simulation are possible at nearly every position of the program and even the structure of the model is modifiable, while needing a relatively low effort in the programming process. Though, concerning the problems with constraints, it is possible to encounter unsurmountable obstacles while using microscopic models:

In order to meet the constraints, that are normally defined on an aggregated level (budget, pharmaceutical resources, hospital beds etc.) the simulation naturally also has to be intervened on an aggregated level. If the amount of the necessary intervention is not known, because it is implicitly hidden inside the system as a whole and can therefore not be calculated directly through the constraint (compare DAEs with an index higher than 1), there are problems for the simulation. Therefore the treatment of the problem using closed equation-models is preferred, because here sophisticated methods of solution exist.

Furthermore various studies exist, regarding the possibility of calculating large categories of simple microscopic models with macroscopic equations, while accepting an insignificant loss of information. The techniques of this so called Mean-Field-Theory (de Aguiar, Rauch, and Bar-Yam 2003; Boudec, McDonald, and Mundinger 2007; Bicher and Popper 2013) include for example the diffusion approximation(Kampen, N. G. van 1982), classically used when spatial structures of the model have nearly no impact on the aggregated scales, and, building on that, the so called Pair-Approximation(Benoit, Nunes, and Telo da Gama 2006).

3.4.2 Research Questions

Due to the already mentioned problems, the development of mathematical models, that are able to map heterogeneous populations as well as the integration of realistic economic and social boundary conditions for decision making, may contribute significantly to innovative modelling and simulation in health care. One of the aims is to adapt the already established methods that exist to numerically solve differential-algebraic equations in mechanics, to the existing models of the health care system or to develop, if necessary, new methods. Particularly, it would be desirable, on the one hand, to build up a library of equation solvers for these equation systems in health care, which would help to solve a given equation system, by using already existing methods as solvers (Hairer, Nørsett, and Wanner 1993; Eich 1995; Cellier 2006; Hairer, Ernst 2001; Hairer, Ernst 2000). On the other hand, we will attempt to develop an own method to solve this special type of differential-algebraic equation systems.

In order to reach the technological goals aimed at, while developing and implementing consistent and stable methods, the analysis and response to the following question is going to be necessary:

- How can research questions be suitably defined in the future, based on system knowledge, the data situation and necessary decisions?

Processes that determine the importance of factors have to be set. Thereby it has to be stated, that biological and social gender are often of relevance, when the project is developing or modifying health care politics. This has to be studied, before these factors can be excluded (compare: ignoring biological gender), because not all differences in biological or social gender are significant. This is important in order to avoid models that are too complex, and possibly insolvable.

- How can suitable models subsequently be chosen?
- How can already existing data sources be used for the parametrization of the models and how have these processes be realized and defined in the future?

The chosen questions and features of the used models therefore have to take into account the following aspects:

- Are the benefits and the risks in the course of the treatment balanced in a population of mixed gender?
- Can the effectiveness and the security (side-effects) of the treatment be mapped in a differentiated manner concerning gender, in order to analyse indicators for women as well as for men?
- Are there differences in gender, meaning: is the treatment for a specific gender more effective or secure?
- Is the proposed treatment for one of the sexes more decisive, concerning the treatment options for women and men?
- If modelling age, reproductive state, ethnicity etc. is necessary, possible and advisable, is it also sufficiently efficient to analyse the sub-groups? Can effects on specific sub-populations be evaluated? If this is the case, is the definition of the sub-populations even consistent?

The models and methods developed have to be looked at precisely in order to refrain from the following points:

- the assumption that the results for one sex automatically also apply to the other, meaning the reception and calculation of a model in a undifferentiated manner
- creating a norm, that is not representative, like for example the assumption of a male norm concerning a disease, that affects both sexes
- pathologizing normal biological processes, like pregnancy or menopause
- interpreting results in a way that social or biological gender isignored.

Therefore it is necessary that the following mathematical questions are answered:

- Is the given differential-algebraic equation system solvable?
- How can we find consistent initial valuesfitting the given differential-algebraic equation system?

In the case of simulation models, which are defined using differential-algebraic equation systems, the question of clarity and existence of a solution is inevitable, because this influences directly the solvability of a research question. In the given application this decides, for example, if it is possible to meet the set constraints (meaning for example legal directives or a budget limit), subjected to the given conditions of the system. Especially concerning differential-algebraic equations the theory of solvability has to be applied in a complex manner (Rheinboldt 1991; Rheinboldt, Werner C. 1984) and has to be analysed differently in every case.

The automatized finding of consistent initial valuesworks in a similar manner. The differential-algebraic equation systems with an index bigger than one, generally poses a problem, because also the numeric and algebraic algorithms presented in the literature are very demanding in the process of application (Pantelides 1988).

In general a differential-algebraic equation system (DAE) is given by an implicit equation

$$F(t, x, \dot{x}) = 0. \qquad (3.4)$$

If the Jacobian $\frac{\partial F}{\partial \dot{x}}$ is singular, the system of equations is not directly solvable, this means that the system has index greater than 1.

In mechanics the equations of motion are represented by DAEs, which can be derived from the Lagrangian function. The Lagrangian function L is given by

$$L = T - V, \qquad (3.5)$$

where T is the total kinetic energy and V is the total potential energy of the system, see [2]. Using the Euler-Lagrange equations a DAE is obtained, whereby the Lagrangian multipliers represent the algebraic variables of the DAE.

As an example the kinetic and potential energies for a pendulum described using Cartesian coordinates are as follows:

$$T = \frac{v_x + v_y}{2} \qquad (3.6)$$

$$V = -\boldsymbol{g}y \qquad (3.7)$$

Using these energies it can be seen that the equations of motion of the pendulum are given by the following equations, see [3],

$$\dot{x} = v_x \qquad (3.8)$$

$$\dot{y} = v_y \qquad (3.9)$$

$$\dot{v}_x = -Fx \qquad (3.10)$$

$$\dot{v}_y = \boldsymbol{g} - Fy \qquad (3.11)$$

$$x^2 + y^2 = 1, \qquad (3.12)$$

where $\boldsymbol{g}$ is the gravitational acceleration and F is the Lagrangian multiplier, which can be interptreted as a force. Equation (3.12) is the constraint equation. The DAE (5)-(9) has differential index three, as is typical for mechanical systems, which can be seen from the third derivative with respect to t of equation (3.12).

In Healthcare such models would look very similar. The differential variables, in the pendulum example x, y, v_x, v_y, could for example be interpreted as the sizes of different populations or cohorts. The algebraic variable, F or in general the Lagrangian multipliers, could be the part of the budget given to the corresponding cohort or variables that are derived from other restrictions.

As mentioned before there are many ways to solve an DAE with index greater than one. The simplest way is to substitute the constraint equation by one of its derivatives, so the system has index 1. For the pendulum this would mean to replace $x^2 + y^2 = 1$ with its second derivative with respect to t:

$$2({v_x}^2 + {v_y}^2 - Fx^2 + \boldsymbol{g}y - Fy^2) = 0. \qquad (3.13)$$

In theory this approach is correct because a solution that solves the original equation would also solve the new one. But through the differentiation of the constraint information is lost and the numerical solution is "drifting off".

For DAEs of index 3 this problem is solved by the so called Baumgarten method. Here the constraint is not replaced by the second derivative but by a linear combination of the constraint and its derivatives:

$$\ddot{g} + 2\alpha\dot{g} + \beta^2 g = 0. \qquad (3.14)$$

Again if used on the pendulum the following equation is generated:

$$2({v_x}^2 + {v_y}^2 - Fx^2 + gy - Fy^2) + 4\alpha\left(xv_x + yv_y\right) + \beta^2(x^2 + y^2 - 1) = 0.$$
(3.15)

For models in healthcare this approach could be applied if the DAE has index 3. However it could be possible to generalize this method as long as certain stability criteria are acknowledged.

A possible example for a DAE model in healthcare could be:

$$\dot{p}_1 = I - rp_1 - m_1 p_1 \tag{3.16}$$

$$\dot{p}_2 = rp_1 - m_2 p_2 \qquad 3.17)$$

$$k_1 p_1 + k_2 p_2 = C \tag{3.18}$$

with state variables p_1, p_2 (differential) and r (algebraic). The parameters m_1, m_2, k_1, k_2, I and C can be time-dependent but do not have to. The model could be interpreted as two groups $p_1, p_2$of people that get certain treatments. The costs of those treatments are k_1, k_2 and the effectiveness is given by m_1, m_2. r describes the rate of people that change the treatment and the overall cost for the health care system is C. Finally I describes the input of people that are at first always treated with the first treatment.

Due to the fact, that the algebraic variable r is not present in the constraint it is clear that index of the DAE is greater than one. Further analysis shows that it is 2.

As far as we have seen the approach of transferring the DAEs to a new domain seems to be promising. As a matter of fact the described aspects are only the first step of a successful integration. Besides the possibility of comparing the capabilities the most important aspect is the parallel development of professional simulation pipelines.

4 Simulation Pipeline

As a result of the process that systems and problems getting more complex the idea developed to improve the whole process of development and management of simulations. As a first step, we will take a look on the general concept of reproducibility. The following section was written for this thesis and in parallel also for the domain of modelling and simulation in archaeology, where it was published in the book *„Agent-based modeling and simulation in archaeology"* (Popper & Pichler, 2014). For detailed aspects of reproducibility in archaeology refer to the mentioned book.

4.1 Reproducibility

Reproducibility is a core value for using models in big projects. Starting from a view of the whole project lifecycle, parameter and output definition, documentation as well as verification and validation are important aspects. In this section the variety of tasks that can be done to achieve reproducibility are described, to improve credibility of a model.

One of the fundamentals of scientific work is that knowledge should be transparent, i.e. openly available for professional discourse. Aspects from the angle of reproducibility are in this meaning very important, focusing on how to give and gain input from fellow researchers. From the side of the project team, this demands a statement of limitations and assumptions within a model. As a matter of fact, possible shortcomings will be detected and assumptions may be questioned. Reproducibility is a challenging task and can be cost intensive. Thus, all efforts that help to achieve it should be carried out with respect to their benefit. Special attention should be paid to documentation, visualisation, parameter formulation, data preparation (Freire et al, 2012), verification and validation, which will be summarized briefly.

The section starts with a general description of the development process behind a modelling and simulation project. Understanding this lifecycle is a precondition for talking about reproducibility, since one needs to know exactly in which phase what information is produced. The next sections deal with parameter formulation, documentation and verification/validation. These topics help to substantiate that the developed simulation produces reliable and useable results. These can then be used to gain knowledge that confirms hypotheses - rectification - or to identify wrong hypotheses - falsification. Depending on the domain there might be huge collection of hypotheses, due to missing information. As described in chapter 1, there are domains where we mainly have to build on Observations and Characterisation of the system („Black Box" Modelling). In this domain falsification of assumptions and hypotheses can be a good question. What sounds disturbing for classical engineering domains might be interesting for the domains of health system research or archaeology: just to reduce the amount of possibilities.

4.1.1 Lifecycle of a Modelling and Simulation Study

The process of developing a model and implementing it as a simulation can be referred to as its lifecycle. To understand reproducibility requires a careful look at this subject, because we first need to define its basic constituents – phases, contained concepts and resulting deliverables, that are later being referred to. In general, a modelling and simulation project does not evolve in a straight-forward manner, but rather iteratively (in a spiral process): The model/simulation is redefined several times, until it can be determined to work correctly for its preset goal. In that context, it is noteworthy to say that a model is concerned only with a (simplified, limited) portion of reality. Modellers have to make abstractions, assumptions and define boundaries to get to an easier view - though detailed and complete enough for the study question - that is com- putable. That is why the whole process might have to be done several times, until the right assumptions and abstractions are made. We now give a brief description of the basic structure of the lifecycle, before coming to a more narrative description of the same matter. Figure 4.1 presents a generalized view of a modelling & simulation lifecycle on the basis of work done by Sargent (2010), with some slight adaptions as "Decision Support" was added:

- A problem arises and is being formulated as one or more study questions, which guide the development into the right direction. The ultimate aim of the project is to solve the stated problem and answer on these defined study questions.
- In a next step, the system is analysed and modelled, which leads to a conceptual model that can solve the problem and give answers on the study questions.
- The conceptual model is then implemented in some programming language, leading to a computerized model which can either produce new findings (leading to a redefinition of the problem and thus resulting in a new iteration) or produces results that can be validated and verified, thus being credible.
- Using such a credible model, developers, experts and users may produce results that reflect reality within its predictive boundaries and calculate possible scenarios, for decision support.

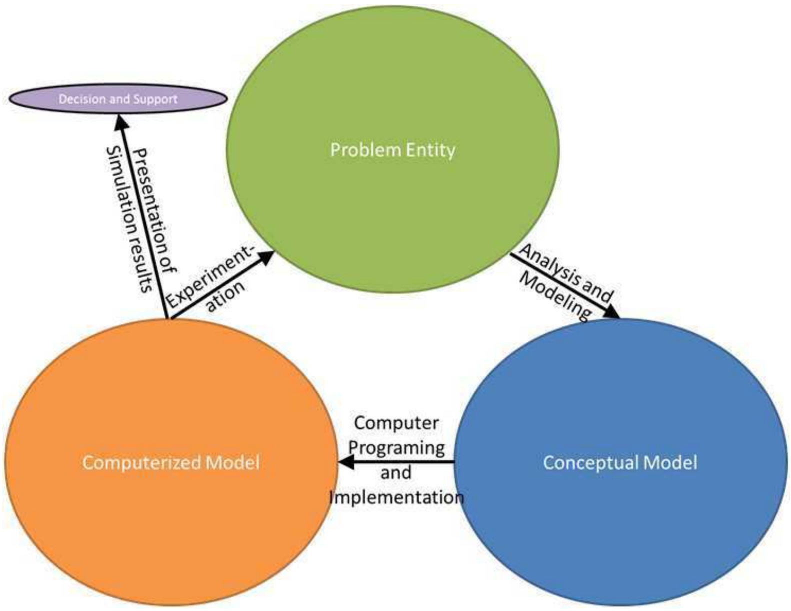


Figure 4.1: Adaptation of the "Generalized Lifecycle of a Simulation Study" by Sargent (2010)

Figure 4.2 shows a more detailed version of the lifecycle, based upon Balci (1994):

- The problem entity phase is split into the communicated problem, formulated problem, proposed solution technique and system and objectives definition.
- The conceptual model phase is divided into the conceptual model and the communicative model.
- The computerized model phase furthermore includes the programmed model, the experimental model and the simulation results.

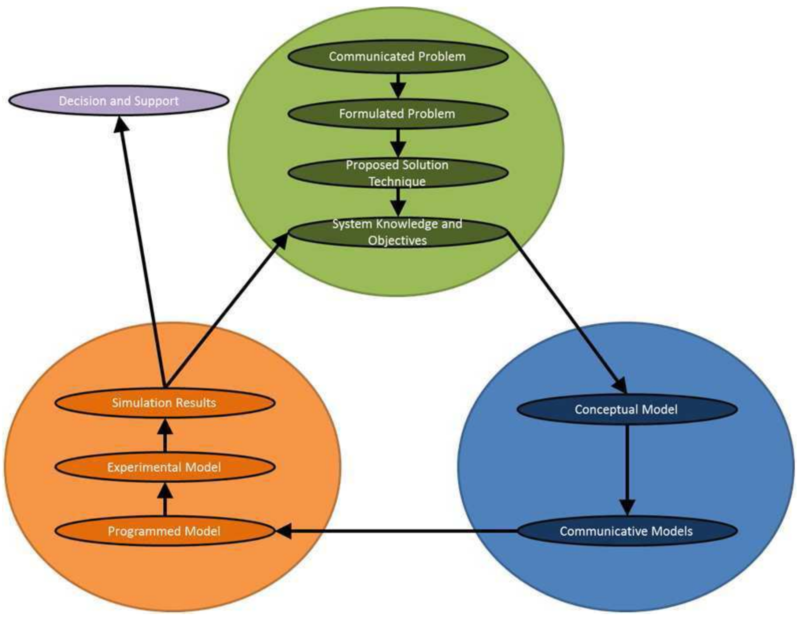


Figure 4.2: Detailed Lifecycle of a Simulation Study, based on Balci (1994)

For better understanding I give a brief example from the chapter "Reproducibility" from the mentioned book *„Agent-based modeling and simulation in archaeology"* (Popper & Pichler, 2014)

Communicated Problem: In the context of campaign analysis, archae- ologists want to look into the process of moving roman foot-soldiers between Messana and Syracuse in the first Punic War (264–241 BC).

Formulated Problem: We formulate the problem as a set of study questions, e.g.: How fast were the foot soldiers marching (time span, speed)? How far in one day?

Proposed Solution Technique: Upon examining the problem closer, we find that it is indeed applicable for an M&S study. Moreover, we opt for agent-based modelling, since the influence of the terrain and the interaction between individuals is probably influential for the overall model.

System Knowledge and Objectives: Foot soldiers marched as a legion of approximately 4800 soldiers. The line-of-flight distance between Messana and Syracuse is 100 km (assumption). By foot, this distance depends on the terrain (which is taken from Geographical Information System).

Conceptual Model: With the given prior knowledge, the modeller thinks of an agent-based model in which a legion is represented as one agent. The terrain is represented as a discrete grid, with a large cell size (50m x 50m).

Communicative Models: We prepare two different models in written form: 1.) The mathematical view on the problem, intended for later implementation and 2.) the archaeological view, intended for discussion. The first contains a description of movement rules, speeds and interaction specifications between legions (there might be more than one), as formulae and definitions. The second communicative model gives a run-down of archaeological descriptions and mental models, which were used as basis for the formulation of the mathematical model.

Programmed Model: Based on the mathematical communicative model, a programmer implements a simulation in Java.

Experimental Model: Together with archaeologists, the modellers de- fine several scenarios (i.e. sets of different parameter values). The simulation is then executed multiple times with these.

Simulation Results: Executions of experimental models lead to results, which (in this case) are given as spreadsheet. These are then subject to interpretation (e.g. in comparison to historical data on this campaign), in order to find out if the results are reliable.

After this step, the lifecycle may re-iterate (refinement). If refinement is not needed, then the results can be taken as current working model (see step "Decision Support" in Figure 4.2). Each part of the lifecycle has its own data and information requirements and leads to a certain generated output. What we really "reproduce" is the output at some stage of the lifecycle, and thus, a closer view is given in the next section.

4.1.2 Parameter and Output Definition

The basis of every Modelling and simulation study lies in the information on which it is based (e.g. studies, databases, expert knowledge, statistical evaluations). In this context, we may differentiate between data and general information: Data contains all quantifiable information and is characterized as having a high degree of objectivity (e.g. as in values within a database). General information is the conglomerate of non-measurable information and has a high degree of subjectivity (e.g. expert knowledge). Regarding the lifecycle presented before, we may say that in each of its stages, a model/simulation transforms data and general information into an output, which is used by subsequent stages as input (see Figure 4.3).

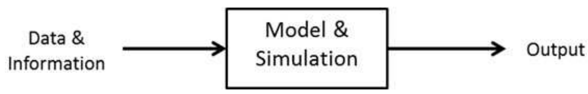


Figure 4.3: Model and Simulation: Data and Knowledge to Output

Data and general information enter the model in the form of parameters (The term "parameter" is used in different meanings across the disciplines. In this chapter, the mathematical / computer science view is presented), through a transformation process: When thinking of the whole modelling and simulation lifecycle, each of the models contained in the different stages demands different parts of the data/information present (see Figure 4.3). The subsequent "execution" of the model at a specific stage may not be a "simulation run" in the sense of a program execution. Rather, it may involve knowledge building and crystallisation (as for example in the Systems Knowledge and Objectives phase), resulting a derived output that is fed into the next stage. Characterizing this even further (and with a view towards Agent-Based Simulation), we can say that each is carrying a name (e.g. "walking speed"), a data type (e.g. a number or Boolean), a range (e.g. 0-2 m/s) and a value (1.4 m/s). For the latter, we may further observe that:

- A parameter's value is constant during the execution of a simulation: For example, one might specify a walking speed for all agents that the simulation will use directly. But one might also specify this walking speed indirectly, giving minimal and maximal walking speeds (both are parameters in this case) from which the simulation will derive the actual speed for each individual agent from a distribution (e.g. uniform distribution, normal distribution. Furthermore, a distribution might be discrete or continuous).
- A parameter's value is variable before the execution of a simulation: It might be changed to experiment with different settings of the model, resulting in different outputs (always the same output for the same parameter settings: deterministic model; different outputs for the same parameter settings: stochastic model).

The set of all possible parameter settings is called parameter space. The act of choosing a value for a parameter is either called parameterization and calibration: In the first case, we make a (hopefully well-informed) choice of a value, whereas in the second case, we pick the set of parameter values that have shown to be in good agreement with the reality that the model is concerned with. Put differently, parameterisation is done a priori and calibration a posteriori. Similarly to the specification of parameters, outputs also need to be defined. For example, we may derive trajectories from a walking model, if the model is sufficiently detailed to be credible. We may also employ different representations for the same output. In the walking model, we may represent the trajectories in a more abstract fashion, using path-time diagrams, or very concretely, by superimposing paths on a map. This aspect rather belongs to visualization, which is elaborated in due course.

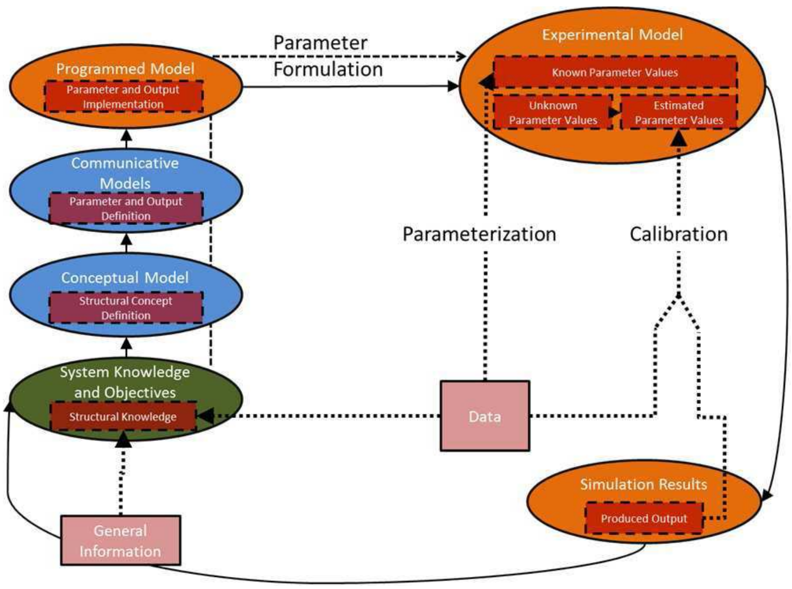


Figure 4.4: Parameter Transformation, Parametrisation and Calibration

Figure 4.4 shows an extended version of the lifecycle presented earlier, with emphasis on definition and transformation of parameters, their parametrisation and calibration:

- The modelling lifecycle begins with the collection of general information and data. Both contribute to the System Knowledge and Objectives phase, in which they are transformed into structural knowledge about the system in question. Interestingly, the data values themselves are not important at this stage; the only thing that is important is to determine which information could be useful for the model (i.e. a first step towards defining its boundaries).
- For the conceptual model, the modeller thinks of a structural concept, separating structural knowledge into information that the model needs or produces. In other words, the modeller tries to establish the dependencies between the types of information that the model will likely use. A detailed definition of this information in the form of concrete parameters is, how- ever, deferred to the communicative models (there might be several, as mentioned, each serving one specific audience): Guided by the gathered general knowledge and the format of the data, this phase produces a well- defined (minimal) set of parameters that can answer the problem. In that context, abstractions and generalisations are applied. For example, walking speeds might be assumed as uniform, if modelling soldiers marching in unison.
- Once proper communicative models with a minimal set of parameters and outputs have been developed, the implementation can start. The resulting programmed model transfers the (mathematical) notion of parameters and outputs into programming-language specific constructs (for example, the Boolean values given as "yes" and "no" are mapped to "true" and "false" in the source code).

At this point in the lifecycle, the implementation has the capabilities to run a simulation. However, we will likely not sweep through the whole range of parameter values possible. Rather, it is necessary to first find reasonable parameter values: The model is subjected to experimentation for exactly this sake, and becomes the "Experimental Model". Depending on the type of parameter under consideration, there are two different techniques for doing this:

- Parameterization (known parameter values): Parameter values can be derived from (a priori known) data values. If the data cannot be transformed in a way that all parameter values can be inferred, further investigations are needed (i.e. broadening the scope of the data basis, gaining new data by conducting experiments, etc.). If this is not possible, some parameters have to be calibrated.

- Calibration (unknown parameter values): Values for unknown parameters are estimated, assisted by given data (statistical evaluations, studies or previous simulation runs). After the experimental model is run, the simulation output is compared to a possibly known output data or, as is often the case in archaeology, to constraints governing the output. If the simulated model produces an output that seems reasonable, the calibration task is finished and the parameter values are - in the best possible scenario - known. If on the contrary the simulation output does not fit, the unknown parameter values have to be estimated again and the experimentation process reiterated (This task is often supported by mathematical optimisation). If calibration fails, a redefinition of the model might be necessary and/or one of the known parameter values has to be doubted. The modelling process starts all over again, because the system knowledge might have changed.

Arguably, the act of calibration is a positivistic, and thus not suited for domains, where we do not have data to fit against. Nevertheless, imposing constraints on what could be an output is in line with what the social sciences would consider a contribution in the first place; in that sense, we argue that the purpose of an modelling and simulation study in this domains lies not primarily in the generation of results per se, but in an exclusion of unlikely scenarios that would otherwise enter the scientific thought process, leading to wrong conclusions. The definition of constraints is a positive "side-effect" of performing such a study, and may in fact lead to the realisation that a previously well-understood problem needs to be re-examined and clarified.

4.1.3 Documentation

Reproducibility is strongly connected to documentation. While it might be easy to say that "all tasks that are important during the development of a modelling and simulation study should be written down", finding a way in which to represent a modelling and simulation study both accurately and efficiently is hard. There are at least three forms of documentation to choose from:

Textual documentation, illustrations and, not surprisingly, the source code itself. We will now look into each of these three categories, giving an overview of techniques that might help in that context.

Textual Documentation

Probably every model author will have his own advice on how to produce textual documentation. Some examples that we found useful are:

Adequacy and Structure: The level of detail in the documentation should be proportional to the importance of the documented entity. Figure 4.5 gives view of the authors concerning the relative importance of each part in the documentation of a modelling and simulation study. Highly detailed topics should be structured into a hierarchy of gradually increasing complexity.

Simplicity: Whenever possible, documentation should be done in Basic English (Ogden, 1940, 1968), a constructed language of 850 words which has a simplified grammar and is designed for the communication of complex thoughts. As a matter of fact, Basic English is easily translated (manually and automatically) and can serve a large international community as a basis for collaboration.

Clarity: A glossary or definition part may help to avoid ambiguities and shorten the text. However, this also carries the risk of over-formalisation. Examples can help to lighten up the text and illustrate an idea intuitively rather than formally.

Audience: Who needs to know what? There are several roles within an modelling and simulation project (e.g. users, model developers), each being interested in a different aspect.

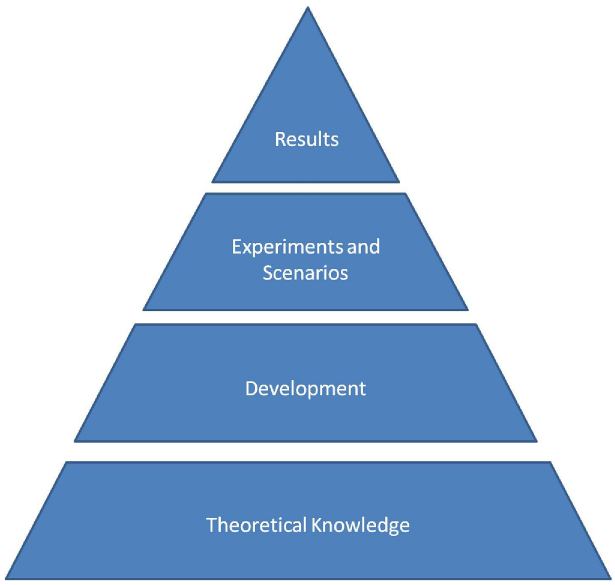


Figure 4.5: Documentation Hierarchy

In addition to these general observations, there are also very specific guidelines for preparing documentation. A widely known example is the ODD (Overview, Design concepts, and Details) protocol by (Grimm et al, 2006). We now come to a short description of its contained parts, according to the first revision given by (Grimm et al, 2010; Polhill, 2014):

Purpose gives a very short summary of the intent of the model.

Entities, State Variables and Scales names the types of agents or cells and their state variables. Furthermore, the spatial and temporal scale of the model is described.

Process Overview and Scheduling describes how the model is updated in each time step, preferably using pseudo-code. The authors also recommend including a description of execution order (when multiple agents are involved).

Design Concepts consists of eleven sub-parts, some of which can be left away for small models or models in which they are not applicable: (1.) Basic principles outlines general concepts behind the model, (2.) Emergence gives a description of overall behaviour arising from the combination of individual behaviours, (3.) Adaptation states how individuals react to changes in themselves or their environment, (4.) Objectives gives a description of the goals followed, either by each agent individually or by a whole team of agents, (5.) Learning describes the change of adaptive traits as consequence of gained "experience", (6.) Prediction gives details over how agents judge a model's future state, (7.) Sensing gives an account of what internal and environmental state variables individuals can perceive and consider in their decision process, (8.) Interaction describes how agents affect each other and the environment, (9.) Stochasticity explicitly states if the modelled processes include a notion of randomness, (10.) Collective gives details over how aggregates of agents are formed and (11.) Observation states what data are collected from the model.

Initialization is concerned with the initial state of the model.

Input data lists required data from external sources, such as files, databases or other models.

Submodels lists all processes briefly outlined under Process Overview and Scheduling, in full detail, including parameterisation and an account of how such a sub model is tested.

According to (Grimm et al, 2010), ODD can be overdone for very simple models. In this case, the authors propose to shorten the documentation "such as by using continuous text instead of separate document subsections for each ODD element".

Source Code

Source code has two great advantages: (1.) It is already there, i.e. there is little overhead in making it "documentation-ready", and (2.) it is automatically kept synchronous to the model (as opposed to every other form of documentation, which needs to be updated to reflect changes). The term "documentation-ready" does not refer to commenting, as comments get out- dated when the model (and thus: the code) changes. Rather, we argue that the source itself is a form of documentation, if written narratively. Some aspects of this endeavour are: (also refer to Martin, 2008)

Choosing proper names: Variables, functions, classes and packages should immediately reveal their purpose through their names.

Do One Thing Principle: Functions and classes should do one thing only (single responsibility), as expressed by their name. Whenever this does not hold, the model developer needs to split and recompose them (thus im- posing a hierarchical structure where code one a higher-level defers lower- level responsibilities to subclasses or functions implementing lower-level behaviour).

Don't Repeat Yourself Principle: Generalising pieces of code that are sim- ilar, using concepts from Object Oriented Programming (i.e. inheritence, interfaces, etc.), makes code easier to read, extend and fix.

When adhering to these concepts, code published online (using for example www.openabm.org) can be understood by a large community of researchers, bypassing the need for secondary literature about the inner mechanics of a model to a certain extent.

Visualisation

Besides textual documentation, visualisation is crucial when trying to document and validate simulation models and thus make them "reproducible". In contrast to source code, which is the most immediate way to communicate the implemented model, the process of modelling and fundamental structural ideas concerning the model can often be better presented via visual concepts.

For a long time, visualisation was restricted to a very small range of possible applications in modelling and simulation: *"[. . .] visualisation was limited to static images until the end of the twentieth century. This explains why visualisation was—and mostly still is—used as a post-processing step with the sole purpose of presenting results. On the other hand, increasingly powerful computers and display devices permitted to move from static images to (interactive) visualisation which has become a field of research in its* *own right"* (Piringer, 2012). In the following section we follow the ideas of this work. Various parts described in this chapter, like the lifecycle itself, parameter- (input) and output definition and analysis or the later-described validation can be visualised. More specifically, one may depict (1.) the model structure, behaviour of agents and so on, typically using vector drawings for rendering graphs and diagrams (as for example in the Unified Modelling Language, (Booch et al, 2005). One may (2.) also visualise a simulation's runtime state (raster graphics showing agents and cells, (Kornhauser et al, 2009) for an extensive treatment on that subject) and to show its results; this is especially helpful in validation, as one can show runtime effects of the model. In addition, data used for the process of parametrisation can (or should) be analysed via "visual analytics", a new field which seeks to get "insight, not numbers" (Hamming, 1962) by employing a variety of depictive techniques. And (3.), quite importantly, one may also communicate the development process of a model visually. Let us give a short glimpse of the possibilities that visualisation offers in the context of reproducibility (concepts are mentioned in the order as they appear in the modelling and simulation lifecycle):

Data Analysis: Visualisation can support archaeologists and modelling experts in their collaboration. Visual analytics helps to analyse basic data, in order to support the detection of relationships and structural errors in the data. More precisely, "visual analytics combines automated analysis techniques with interactive visualisations for an effective understanding, reasoning and decision making on the basis of very large and complex datasets" (Keim et al, 2010). But visual analytics is not an end itself; it is the employment of complex datasets that makes the analysis of multivariate data (as base data) necessary. In that context, one needs to define, calibrate, and validate a model and should also represent the coverage of the parameter space adequately (think: depiction). Time-dependent datasets are special cases of complex datasets, which serve as longitudinal base data (e.g. harvest yields, periods of illnesses) in the context of archaeology. Using visual analytics on that data supports hypothesis generation, intuitive integration of domain knowledge and also helps to make complex and unclean data nevertheless applicable.

Modelling Process: The process of building models is highly iterative. Starting with data analysis and the generation hypotheses, it extends over the whole lifecycle and evolves in a spiral process. Research in interactive model building (Bertini & Lalanne, 2009) aims to tightly integrate (1.) the specification and adaptation of models with (2.) an evaluation of results, in order to obtain well-understood models with less effort. Visualisation can aid in this process and, by doing so, also increase reproducibility. One specific example for that would be the visualisation of different parameterisations during the modelling phase: For example, reflections on inherent uncertainty in the parameters can be done when multiple simulation runs enable the modeller to sample the distributions of one or more parameters, in order to determine the uncertainty of the outputs (sensitivity analysis). A visual characterisation of both parameter and result space helps to identify all possible results that a particular model may possibly generate, and thus helps to simplify a model by omitting ineffective parameters. Furthermore, visualisation in the context of the modelling process can also help in calibration.

Structure: Assessing visualisation approaches for representing a model's structure includes a high number of technologies, like visualisation of trees and graphs. Visualisation concepts for these models are well known. ABMs are a flexible, general approach. Thus, a detailed projection of those structures onto the model leads to a wide variety of model types, as agents can represent moving armies, vehicles on roads or something completely different. Different agents, different interactions, different rules and different structures make it almost mpossible to provide a generally usable visualisation technique. Today, most visualisations of agent-based models focus on the model structure (especially the agents themselves), their behaviour and their interactions. (Kornhauser et al., 2009) have proposed some guidelines for visualisation design specifically for agent-based modelling, which can be used to identify important model elements and help users to understand the model's behaviour.

Runtime & Results: Visual representations of simulation results include general-purpose statistical plots like bar charts and scatter plots (Tufte 1983) as well as diagrams addressing specific questions of the professional field . Techniques of visual analytics can be used for visualising (potentially very long) time-dependent data of single time series as well as a large number of time series of simulation results. Agent-based simulations constantly produce new data with every time step. A potentially large number of agents makes it difficult for the user to keep track of a particular agent or group of agents' position, colour, size, or shape. In this context, Healey and Enns discuss common visualisation tasks such as target and region tracking, boundary detection, and estimation and counting (Healey & Enns, 2012). However, visual summaries of a simulation run are often far more effective for analysing the model and its implications than a look at individual agents. There are several examples over well-established techniques in that context (Tufte 1983, 1996, 2006), however, such "simple" depictive tools may get more complex once "drilling down" into the information. An example of such a "complex summary" could be a social network analysis reflecting the contact and interaction between agents.

Also, note that visual analysis can also be used for excluding certain hypotheses (rather than proving with reference to some data). In that sense, one can look at different scenarios (representing the hypotheses) and scrutinize the underlying data (visually), in order to save modelling efforts if a scenario can be easily rejected.

Verification and Validation

Verification answers whether a model is implemented correctly, i.e. *"Is the model developed right?"* Validation addresses the problem whether a model is able to answer a specific research question: "Is the right model developed?"

Both can be seen as processes that happen in parallel to the development of the model and the simulation. Their aim is to guarantee a targeted development of the simulation study. Another important term connected to verification and valdiation is credibility. According to Law and McComas (2009), *"a simulation model and its results have credibility if the decision-maker and other key project personnel accept them as correct."* The higher the degree of scrutiny within the development process, the higher the possibility that the model is credible. But, *"note that a credible model is not necessarily valid, and vice versa"* Law and McComas (2009, p.23).

In most cases verification and validation is carried out by the development team itself. The downside of this approach is that developers may tend to follow the same procedure that they use for development when they verify (i.e. they are caught in the same tracks). A better way is to conduct verification and validation by an independent third party (e.g. a "Verification and Validation Task Force", consisting of a mixture of people familiar with modelling and people connected to the field of study).

In the following, we give a description of verification and validation in respect to the generalized lifecycle (see Figure 4.6).

Conceptual model validation happens in the analysis and modelling phase. All abstractions, theories and assumptions are checked using mathematical and statistical methods.

Computerized model verification deals with the substantiation of the right programming and implementation of the conceptual model. Different programming languages offer a broad variety of concepts to do this.

Operational validation deals with the evaluation whether the model parameter is chosen right in respect to the purpose of the simulation. Here the biggest part of the validation takes place. It is important to remember that mistakes that are found in this part of the modelling lifecycle can either be mistakes that were either made in the analysis and modelling part or in the computer programming and implementation. The best way to do operational validation is the comparison to the real world problem. If it is not possible to do this, a comparison with other models should be done.

Data validation helps to determine whether the data is correct. If assumptions are made to use the data, it helps to determine whether these are proper assumptions.

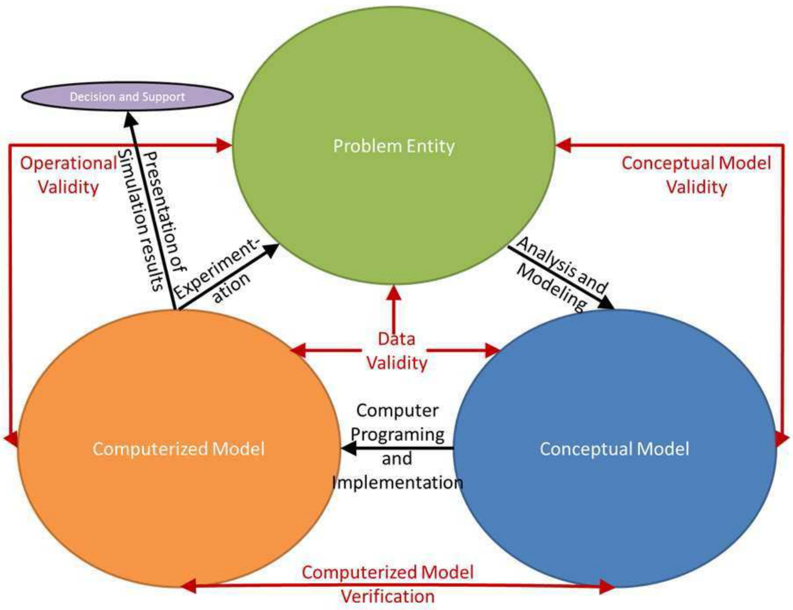


Figure 4.6: Verification and validation in the generalised lifecycle of a simulation study

Arguably, the most simple validation technique is the plausibility check: It is an evaluation over whether the produced output is comprehensible, if the parameters are known. This can be done by either comparing the results to reality or, if that is possible, to other simulations. Another possibility in that context is to use expert knowledge. However, there are many more techniques like this, as is shown in due course. According to Balci (1994), these can be classified into six groups:

Informal Techniques: Techniques that rely on subjective judgement. This does, however, not mean that there is a lack of structure or formal guide- lines being used in this case. Some examples also applicable to agent-based simulation are:

- Audits: A single person evaluates whether the simulation study is done in a satisfying way (e.g. checking whether it meets the preset requirements). As a byproduct, errors and mistakes may be uncovered.
- Inspections, Reviews, Walkthroughs: Each of these methods involves a group of people which is trying to evaluate whether the development

is done in a satisfying way. These methods aim at different parts of the mod- elling lifecycle and use a variety of instruments.

- Turing Test : This testing technique was invented in 1950 by Alan Turing: A computer program is said to succeed the Turing Test if a real person cannot figure out whether the results are produced by a program (in this case: the simulation) or the results are taken from the real system.
- Face Validation: An expert checks whether results are reliable and reasonable. Results of other validation and verification strategies might support the expert in his decision.
- Desk Checking : The work of each team member is checked for correctness, completeness and consistency. As a side-note, model developers should not do desk checking by themselves, because mistakes are often overlooked or disregarded.

Static Techniques: The source code (which does not need to be executed, mental execution is enough) is automatically analysed by a compiler. To give some examples, consistency checking is a pre-step to compilation that can ensure a common programming style among the developing team. Syn- tax analysis is the basic compilation task can find wrongly spelled or gram- matically wrong language constructs. Data flow analysis can furthermore detect undeclared or unused variables.

Dynamic Techniques execute the model and analyse its resulting behaviour:

- Sensitivity analysis analyses the impact of parameter changes on the out- put, by comparing multiple simulation runs in which parameter values have been systematically changed. An expert then has to check the re- sults of this comparison. For example, a model that is very sensitive to input changes might easily lead to wrong results (or accumulated effects thereof), if the input data and parameters are not well-controlled.
- Black-box Testing : Input parameters are fed into the model and the accuracy of the output is evaluated without looking what happens inside the model.
- White-box Testing : This is more a verification technique than a validation technique, which we mention here for the sake of completeness. It is the same as Black-box Testing, albeit with access to

the underlying code. Because this is known, a test run can demand for example that the whole code needs to be covered by a specific test. Or, it could demand that as many different logical conditions in the code are to be covered as many times as possible, thus substantiating the accurate operation of a simulation.

- Bottom-up Testing : This validation strategy is possible for simulations that are developed in a bottom-up manner: After sub-models are developed, an integration test is performed: This starts with the most basic functionality (e.g. simple movement of an agent), goes on to aggregate level (e.g. steering behaviour of an agent) and continues onto the topmost level (e.g. movement of a crowd).

- Top-down Testing : This validation strategy is possible for simulations that are developed in a top-down manner. It is the counter-part of bottom-up testing: After a top model is completely developed, a hierarchical integration test for the sub-models is performed.

- Graphical Comparisons: Real-world data is compared to the modelling variables and parameters, assisted by graphs in which e.g. linearity, exponential or logarithmical rise, periodicities and so on are analysed. Such comparisons can furthermore be used not only for checking against real- world data, but also against other models.

- Visualisation: The simulation output is visualised through the whole simulation run. This technique can only be seen as validation strategy if the results are checked for plausibility afterwards.

- Predictive Validation: The model is fed with known (past) input parameters. The model output is then compared to the real world behaviour. Of course, this can only work when real-world data (both input and output) is at hand.

- Statistical Validation: A model could be statistic validated when the system is completely observable. For example, variance analysis, confidence intervals and so on may be done for the output. Whether this is a good validation strategy or not depends on the inner mechanics of the model. It is thus important to use many different data sets to see whether the statistical statements deduced are always the same, and the technique can therefore be applied.

Symbolic Techniques are for checking cause-effect relationships (through graphs), checking functional correctness of each part of the simulation (this is also called partition testing), testing specific portions of a simulation by supplying it generated test data that should cause a certain execution (path analysis), and lastly symbolic evaluation that tests all evaluated paths in a program to find out if some are unnecessary or incorrect. In later work (Balci, 1997), this category was incorporated into the dynamic and static techniques.

Constraint-Based Techniques: Supported by constraints, model correctness is warranted. These constraints can be seen e.g. as run-time assertions, which ensure that the simulation stays in a well-defined state. Balci (1997) gives this category up completely, and incorporates these concepts into the other categories.

Formal Techniques: Mathematical deduction and other formalisms are used to e.g. check the correctness of the simulation. As Balci (1994) admits, *"Current state-of-the-art formal proof of correctness techniques are simply not capable of being applied to even a reasonably complex simulation model"* (Balci 1994). Especially for agent-based models, formal techniques are still in a very early stage, and a general formal approach (for all scenarios where agent-based models are used) is still beyond the current state of the art.

Verification and Validation for Agent Based Models

Agent-based models are characterized by a complex behaviour that cannot be entirely observed. This is why informal techniques can always be used, because these are subjective methods. Methods with a very formal background, as already stated by Balci (1994), cannot be used for the entire model, due to high amount of complexity involved. But even when some parts of an agent-based model can be formally validated, this does not imply that the composition of all parts is also valid.

One specific "agent-based" validation strategy is called Immersive Face Validation (Louloudi and Klügl, 2012). It is a strategy in which one tries to see the model as from an agent's point of view. Thus, the path of an agent is tracked through the whole simulation. It is then analysed and checked against the model's assumptions, using a virtual environment (i.e. 3D visualisation) in which the behaviour of one particular agent can be assessed. As the authors state, "after completing one full simulation run, the evaluator should describe the overall comments briefly in a post processing activity and reply on model- specific questionnaires" (Louloudi and Klügl, 2012) . According to the categories described earlier, this is thus an informal technique.

A procedure for the validation of an agent-based model, based on Klügl (2008), is shown in Figure 4.7: The authors assume that the model has already been subjected to a conceptual model validation and is now ready for execution ("Runable"). This execution is assessed using a face validation, leading to either a sufficiently plausible model or a re-iteration ("not sufficiently valid"). The plausible model then undergoes a sensitivity analysis, which leads to an assessment regarding which parameters are influential and which ones are without effect. The latter ones can be deleted (together with code parts connected to them), leading to a "Minimal Model". Then comes a calibration part, in which parameters have to be set such that the model produces valid results. Note that the calibration process itself is not a validation method - it is merely a part of that procedure. A following plausibility check is then conducted, which is "basically the same as the previously discussed face validation, yet may not be executed as intensively as before as we assume only limited changes in the simulation outcome" Klügl (2008, p.43).

Additionally to mention is the work of (Muaz et al, 2009), who have introduced an approach called VOMAS (Virtual Overlay Multi Agent System): Special agents - so called VOAgents, monitor the agents of the simulation ("SimAgents"). This VOAgents can get simple rules which tell them what to do, for example rules that tell them to trace single Sim- Agents, log SimAgents with certain attributes or variable values and so on. Also, groups of SimAgents with certain attributes or variable values can be monitored in that manner. Basically it is an extended and individualized protocol module with a high degree of flexibility, if implemented right. This system can be used to support the validation of agent-based models within the same environment. Thus, care has to be taken that VOAgents are really only "external observers" and not influencing the model's state.

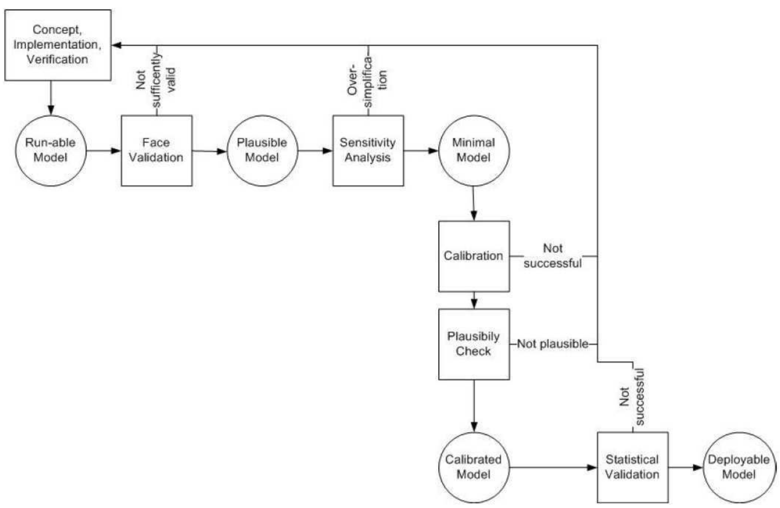


Figure 4.7: A validation methotology for agent-based simulations, based on (Klügl, 2008)

Additional aspects not covered are how a model structure can be communicated, for example, given by the ODD protocol (Grimm et al, 2006) and legal aspects of communicating model structure, as covered e.g. in (Stodden, 2010).

4.2 Falsification

A special aspect resulting from the considerations on reproducibility is the definition of the research question "falsification". Scientists usually want to test one or more hypotheses. The first thing that comes to mind when thinking about a successful simulation study is that the simulation has to have an outcome that helps to confirm these hypotheses (i.e. an expected outcome).

But simulations can also be used to gain more knowledge about the system under study: It can prove whether given assumptions or abstractions might be wrong; by falsification, it helps to reduce the number of possibilities to the ones that seem reasonable.

As an example the prehistoric salt mines of Hallstatt in Austria are presented. They are subject of great interest for archaeologists, as there is a large amount of archaeological findings of technical equipment and organic materials (timber, wooden tools, strings of bast, fur etc.) The perfect conditions of preservation in the mines due to the conserving properties of salt allow for a reconstruction of the working process in the mines (Reschreiter et al. 2009).

Investigations suggest that mining was organized in an efficient, nearly industrial manner with highly specialized tools. Salt was mined in underground mining chambers using special bronze picks. Typically, experimental methods using reconstructions of historical technologies are used in archaeology to provide deeper insights on technological issues. As a new tool, modelling and simulation can also serve as a method for gaining knowledge in different aspects of archaeology. The group of Hans Reschreiter and Kerstin Kowarik had the idea to test a hypothesis – and maybe to falsify it.

Salt was mined using bronze picks with wooden handle. Highly interesting is the unusual shape of the pick with a typical angle between the shaft and tip of about 55 to 75 degrees. It is believed that this particular shape was adapted to the specific working conditions in the Hallstatt mines, especially since no similar devices have been found at other at archaeological sites. The small angle does not allow typical circular hacking motion, which is why it is not yet completely clear exactly how such a pick was used.

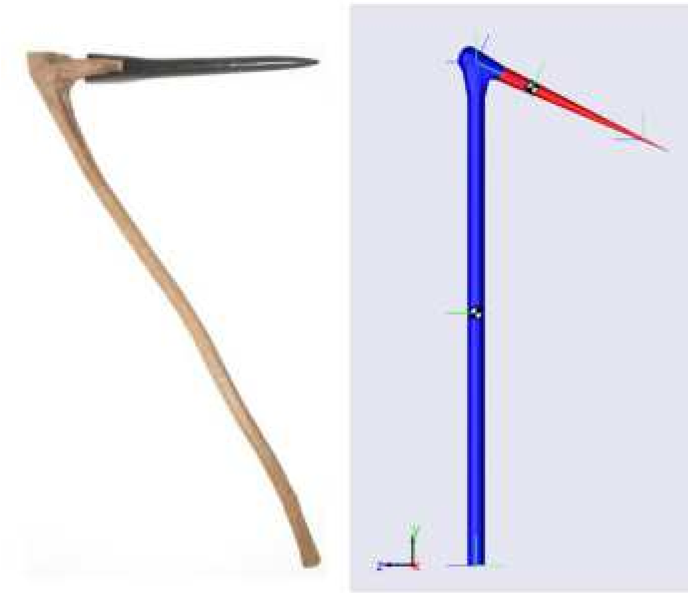


Figure 4.8: Left: Reconstructed Bronze Age Pick (© A.Rausch, NHM Vienna). Right: Rigid Body Model of the Pick in MATLAB/SimMechanics by B. Heinzl et al

Modelling of the pick as a rigid body system allowed evaluation of possible movement scenarios and comparison regarding resulting force and momentum on the tip. Several points were defined along a trajectory of the tool tip depending on the range of motion for a human and a special focus was put on the angle, in which the tool tip hits the ground.

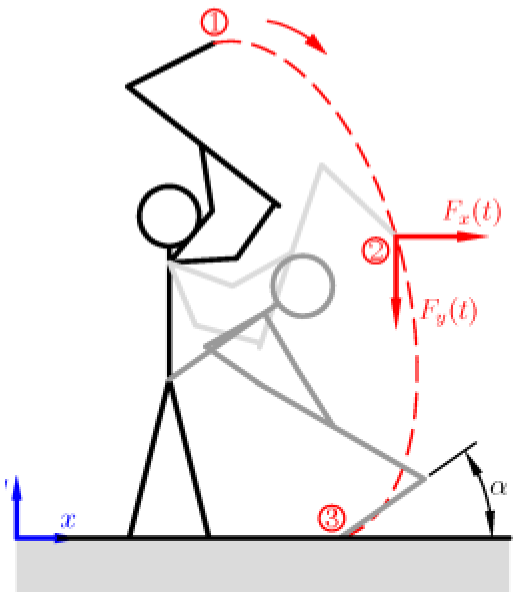


Figure 4.9: Trajectory for Movement of the Tool Tip and Reaction Forces F_x and F_y .

With the simulation model some assumptions about the usage of the pick could be excluded from further investigations, as the body movement and energy requirement were not possible to be matched with the simulation model.

Based on the successful results, the concept of falsification was - based on Reschreiter and Kowarik and the work of Gabriel Wurzer - also successfully applied on agent-based models for the Hallstatt archaeological site (in publication).

Definition 4.8 (Falsification). Falsification is the evaluation of simulation studies to exclude a Model or a Parameter/Input Set of a Model of further investigations.

However, falsification may also be hard to achieve: "If the model contains too many degrees of freedom, an automatic optimizing calibration procedure will always be able to fit the model to the data" (Klügl, 2008). As example for a model in which falsification was expected but not manageable, the author names the EOS project Doran and Palmer (1995): *"Two competing plausible hypotheses for explaining the emergence of social complexity were simulated, both were able to reproduced [sic!] the observed emergent structures. Thus, no theory was rejected, the modeller had to admit, that without additional data no discrimination between the two hypotheses could be made"* (Klügl, 2008, p.41).

There is no single point at which a model – especially an agent-based one, can be made "reproducible", "validatable" or "falsifyable" (all of these terms are properties and not tasks to conduct). Instead, we have to look at the whole lifecycle of an modelling & simulation study and address aspects such as documentation, verification and validation, which were presented herein. It is also clear that these need to be carried out throughout the entire development process. Moreover, as initially stated, the knowledge produced in such manner should be transparent, i.e. openly available for professional discourse and scrutiny. Another special aspect of using innovative concepts of modelling and the simulation processes with different modelling methods will be presented in the next section:

4.3 Cross Model Validation

One concept arising from previous considerations is doing validation between models, by comparing different models between each other, so called "cross model validation".

Definition 4.9 (Cross Model Validation). Cross Model Validation is the comparison of two models of a system to differentiate between system immanent and model immanent effects.

As described the idea of getting different models for the same problem can result in (1) the same outcome or (2) in differences, even if parametrisation transfer was made properly. This might happen, if the model shows model immanent effect like spurious invariants in LGCAs (Succi, 2001) or system immanent. In the first case we could find it out, based on the concept of Cross Model Validation. Another reason for introducing the concept of cross model validation are systems, where validation is not possible, like interventions in the health system.

The concept was first applied for the modelling of a vaccination strategy to prevent pneumococcal disease and was published by (Zauner et al, 2010 ; Urach, 2009)

4.3.1 Vaccination Strategies against Pneumococcal Infections

Based on definition of CDC (Centers for Disease Control and Prevention) from 2015, pneumococcal disease is caused by a bacterium known as Streptococcus pneumoniae, or pneumococcus. Pneumococcal infections can range from ear and sinus infections to pneumonia and bloodstream infections. Children younger than 2 years of age are among those most at risk for disease. There are vaccines to prevent pneumococcal disease in children and adults.Besides pneumonia, pneumococcus can cause other types of infections too, such as:

- Ear infections
- Sinus infections
- Meningitis (infection of the covering around the brain and spinal cord)
- Bacteremia (blood stream infection)

Some of these infections are considered “invasive.” Invasive disease means that germs invade parts of the body that are normally free from germs. For example, pneumococcal bacteria can invade the bloodstream, causing bacteremia, and the tissues and fluids surrounding the brain and spinal cord, causing meningitis. When this happens, disease is usually very severe, causing hospitalization or even death.

4.3.2 Research question

Based on information of MedlinePlus, a service of the U.S. national library of medicine (NHS), there are 91 strains of pneumococcal bacteria. Pneumococcal conjugate vaccine (PCV) protects against 7 of them. These 7 strains are responsible for most severe pneumococcal infections among children. But pneumonia and ear infections have many causes, and PCV only works against those caused by pneumococcal bacteria. PCV is given to infants and toddlers to protect them when they are at greatest risk for serious diseases caused by pneumococcal bacteria.

Based on detailed data evaluation and a systematic literature research the socio-economic impact of an implementation of PCV7 (heptavalent Pneumococcal

Conjugate Vaccine) vaccination into the Austrian children vaccination program using mathematical models in an HTA (Health Technology Assessment) report is of interest. A major problem and therefore the main challenge is, that on the one hand herd immunity effects against the strains in the vaccine can occur, but on the other hand a possible serotype replacement can happen. The modelling process by its definition has to be capable to integrate these effects into the structure.
Therefore the modelling process has to deal with:

- Natural spread of disease
- Modelling of carrier rates in different age groups
- Influence of different serotypes, summed up as vaccine-serotypes and non-vaccine-serotypes on sever illnesses (meningitis, sepsis and pneumonia)
- Vaccination strategies

Due to expected effects also on non-vaccinated age groups, like the elderly, and long-time horizons till getting full vaccination program effects population dynamics have an influence and have to be modelled.

4.3.3 Modelling approaches

As the modelling and simulation process for Austrian setting has to fulfil

1. Comparability to literature approaches from other developed countries (especially UK), and
2. Depict real world complexity as defined by research question.

The explained modelling techniques used solving the PCV7 research questions described in the following section is also based on (Zauner et al, 2010).

The classical/literature approach in PCV7 vaccination program evaluation

The classical approach using a Markov cohort model is based on one of the first, mainly cited papers on PCV7 children vaccination program evaluation in UK (McIntosch, 2003). It represents the state of the art of vaccination strategy evaluation in a socio-economic setting by a classical HTA.

Hereby the reduction of cases of illnesses due to nationwide PCV7 vaccination of infants and as a consequence therefore cost reduction is realized by a Markov model (Markov chain with one year time step, modelling a whole birth cohort). The model splits in two parts, the counting part of the illnesses and, the cost calculation part.

The model structure for the first part is shown in figure 1.

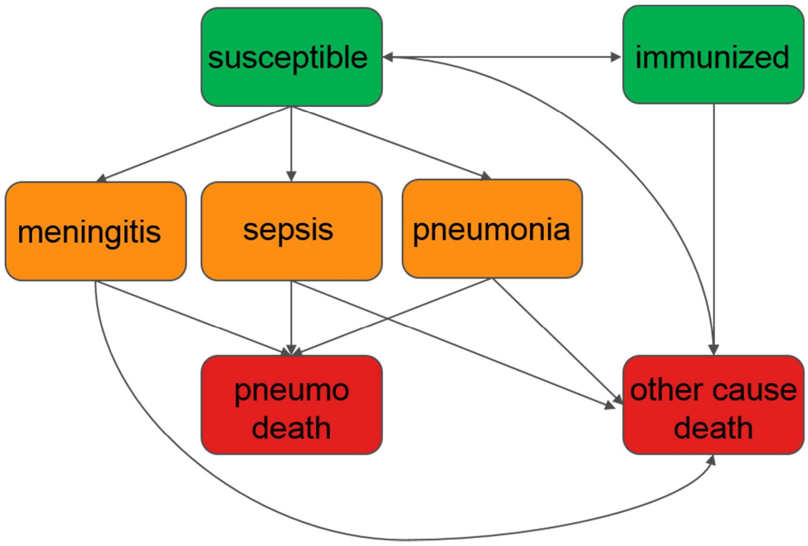


Figure 4.10: PCV7 Vaccination Modell - Basic Model Structure

In this model the dynamic non-linear effects herd immunity is implemented by a fixed factor and therefore the model structure cannot represent different strategies without not verifiable expert knowledge. This implicates low grade of evidence.

Serotype replacement as well as population dynamics and effects on other age groups cannot be realized using Markov Chains, therefore the value of cross validation is poor. The memorylessness of the method is the main reason of these problems. A standard way of fitting these problems, coming closer to real world behaviour uses classical mathematical infectious disease modelling, leading to an ODE approach.

Dynamic modelling approach

Based on identified problems using Markov models for vaccination strategy evaluation for infectious diseases classical mathematical methods from outside HTA with macroscopic view are favourable. ODE fulfil the main demand and solve the problem of memorylessness. A broad spectrum of literature (for example Petrovski) on how to set up an ODE for infectious diseases is published. Main starting points are SI, SIS or SIR models.

Implementing the model by stepwise refinement and data calibration for the classical non-vaccination comparator a model structure results in the following ODE structure:

$$\dot{S} = -S \cdot \frac{b_1 \cdot (I_1+I_{1,2}+I_{2,1}) + b_2 \cdot (I_1 + I_2+I_{1,2}+I_{2,1})}{N} + a_1 \cdot I_1 + a_2 \cdot I_2$$

$$\dot{I_1} = b_1 \cdot S \cdot \frac{I_1 + I_{1,2} + I_{2,1}}{N} + d_1 \cdot I_{2,1} - \frac{b_{1,2} \cdot I_1 \cdot I_2}{N} - a_1 \cdot I_1$$

$$\dot{I_2} = b_2 \cdot S \cdot \frac{I_2 + I_{2,1} + I_{1,2}}{N} + d_2 \cdot I_{1,2} - \frac{b_{2,1} \cdot I_2 \cdot I_1}{N} - a_2 \cdot I_2$$

$$\dot{I_{1,2}} = \frac{b_{1,2} \cdot I_1 \, . \, I_2}{N} - d_2 \cdot I_{1,2}$$

$$\dot{I_{2,1}} = \frac{b_{2,1} \cdot I_2 \, . \, I_1}{N} - d_1 \cdot I_{2,1}$$

$$N = S + I_1 + I_2+I_{1,2}+I_{2,1}$$

The different I subtypes represent the splitting of the serotypes of pneumococci into the ones included in the vaccine and the others. The I therefore means carrier, not equal to the ill persons with symptoms. For disease transmission the carrier status is crucial. The number of severe diseases is calculated out of the carrier rates by using age depended probability functions.

A model structure like the implemented ODE fulfils the research question, but is limited in cases when additional effects like urban/sub urban regions or additional effects on disease transmission with local effects have to be taken into account.

Microscopic modelling

The individual based / agent based approach is one of the standard bottom-up simulation techniques and is the most intuitive approach if communication in interdisciplinary teams with reduced mathematical background is standard. Especially in HTA or EBM (Evidence Based Medicine) setting this happens quite often.

The main field of application in disease modelling is the part when either social interaction can lead to spread of disease or has an influence on disease progression. In case of pneumococci we have an airborne disease and therefore social interaction modelling is the most realistic approach. Agent based modelling using contact networks for social interaction and parameterization of heterogeneous persons performs an adequate computer model of such a complex real world system (additional see "Multi Agent Simulation Techniques For Dynamic Simulation of Social Interactions and Spread of Diseases with Different Serotypes" by (Zauner et al, 2010).

Concrete the Austrian population and its prognosis for dynamics over time as well as the underlying contact networks resulting in carrier rates for the different serotype groups of pneumococci realized based on the structure shown in figure 4.11 are implemented.

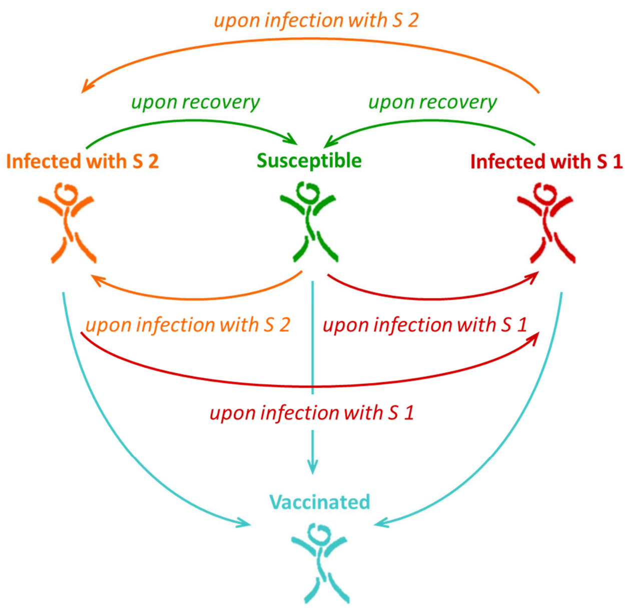


Figure 4.11: PCV7 - Structure of serotype groups of pneumococci

The modelling approach using agent based modelling results in highest flexibility for scenario calculation and meets the real world behaviour best. The standard solution using Markov models are not advisable. Nevertheless the advanced ODE structure also shows high quality results, already evaluated with new data of foreign countries.

4.3.4 Cross Model Validation

In this example additional model concepts were introduced to implement to special effects, which were analysed within the simulation process, especially the serotype replacement. One problem is that there are many uncommon serotypes that are not covered by the vaccine. Some studies presume that vaccinated people get infected with uncommon serotypes instead so other serotypes could become more common. So the real long term effect of the vaccination could be much lower than expected. There is even one clinical study that reports serotype replacement. But usually serotype replacement cannot be observed because at the moment only a too small part of the population is vaccinated and therefore random effects cannot be separated. The few vaccinated people really benefit in many studies because they just do not get in touch with uncommon serotypes and compared to the rest of the population they are not many enough to make uncommon serotypes more common.

The developed model was able to give some more information if such a phenomenon can be expected and how strong it might be. On the other hand via agents a second systemic behaviour could be introduced: Herd immunity. The presumption was that there exist substantial effects for the whole population if only children are vaccinated. The explanation is on the one hand a much higher percentage of children than adults are infected, on the other hand in some studies it is presumed that most transmissions of this pathogens are between infants and adults because their physical contact is often much closer than between two adults.

The comparison of the different models showed very soon, that the systemic effects could be identified within the cross model validation.

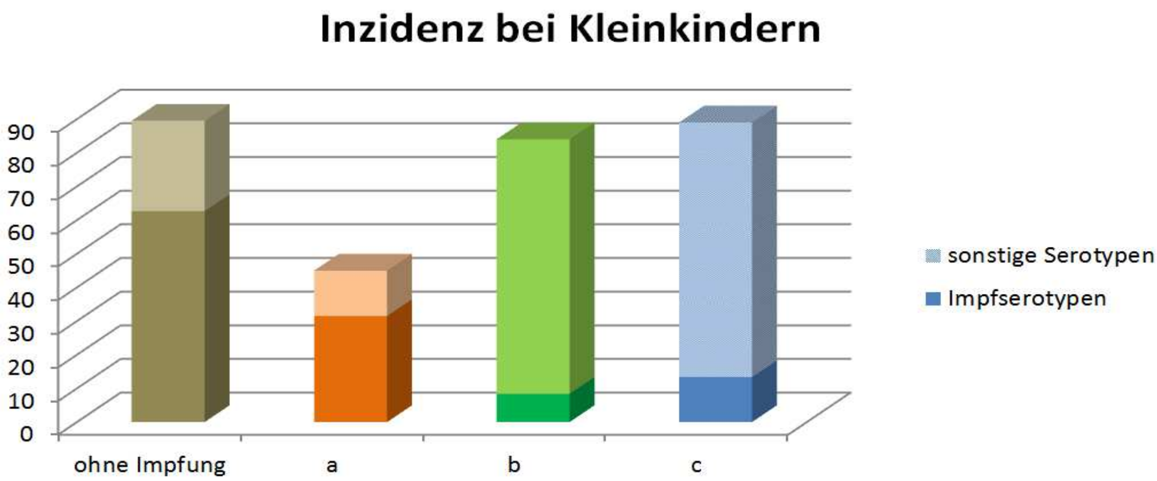


Figure 4.12:PCV7 Result of Cross Model Validation and Systemic Behaviour from (Urach, 2009)

In 2009, when the project was implemented, the actual situation was as shown in the left bar in brown. The classical Markov approach was computed for the UK and was transferred to Austria. *(E.D.G. McIntosh, P. Conway, J. Willingham, R. Hollingsworth, and A. Lloyd. The cost-burden of paediatric pneumococcal disease in the UK and the potential cost-effectiveness of prevention using 7-valent pneumococcal conjugate vaccine. Vaccine, 2003 Jun 2,21(19-20):2564-72))*. Looking at the Cross Model Validation we can see that regarding to the relevant characteristics – serotype shift - the dynamic model could represent the effect much better *(green bar, Urach, 2009)*.). Finally in 2010 results from the United States, where the vaccination was introduced proofed the Cross Model Validation. *(2010 results from USA, applied for Austria :Hsu KK et al. Changing serotypes causing childhood invasive pneumococcal disease: Massachusetts, 2001–2007. Pediatr Infect Dis J 2010 Apr; 29:289)*

Cross Model Validation is now also recognised in the Modelling Good Research Practices approach developed by the ISPOR (International Society for Pharmacoeconomics and Outcomes Research) Modeling Task Force jointly convened with the Society for Medical Decision Making. (Eddy et al, 2015) Here updated recommendations for best practices in conceptualizing models are developed. The Modelling Good Research Practices are dealing with implementing state transition approaches, discrete event simulations, or dynamic transmission models, dealing with uncertainty and validating and reporting models transparently.

"Cross validation“ is here used without „Model“ in between Cross and Validation, which might lead to misunderstandings, as cross validation is also used as name for a validation technique for estimating the generalization ability of a model to an independent data set. It is mainly used in settings where the goal is prediction (age of an archaeological find, the class an object most likely belongs to,...), and one wants to estimate how accurately this predictive model will perform in practice. In a prediction problem, a model is usually given a dataset of known data on which the training is run (called the training dataset) and a dataset of unknown data (or first seen data) against which the model is tested or validated. The goal of cross validation is to define a dataset to "test" the model in the training phase in order to limit problems like overfitting, give an insight on how the model will generalize to an independent dataset.

Nevertheless in our usage it is described in the Modelling Good Research Practices as *"method, which has also been called external consistency and external convergence testing, involves giving the same problem to different models and comparing their results."* …. *"The extent of differences among the models' results and sources of the differences are then examined."* Strengths and limitations of the method are described as follows: *"Confidence in a result is increased if similar results are calculated by different models using different methods."* Limitations are summarized: *"First, this type of validation is only possible when there are multiple models capable of analysing the same problem…. In healthcare modeling there is often a high degree of dependency among models in that they may use similar frameworks and the same data sources. Some models even draw on parameters used in other models published earlier. Similar results could as easily mean that all the models are inaccurate as that they are accurate."*

5 Applications

5.1 A General Concept for Description of Production Plants

The goal of the project BaMa (Balanced Manufactoring) was described in section 1.3.1.. Based on presented methods and technologies application for this project will be outlined, see also prior publication of the approach (Popper et al 2014b). BaMas goal is to develop a simulation-based method for monitoring, predicting and optimizing energy and resource demands of manufacturing companies. The project is funded by the Austrian Research Promotion Agency (FFG, project number 840746) and the Austrian Klima- und Energiefonds (KLIEN). Considering the economic success factors time and costs, a new modelling and simulation concept will be integrated in the research project to implement an energy and cost foot printing. A modular approach that segments a production facility into "cubes" will be developed. Cubes have a clearly defined interface and represent a certain physical behaviour that contributes to the energy balance of the overall system. In this section it will be shown how cubes are defined and how formal concepts for interfaces, system behaviour, and hierarchical layout are described.

Balanced Manufacturing (BaMa, the project is running from 2014 until 2018) will develop a simulation-based tool for monitoring, predicting and optimizing energy and resource demands of manufacturing companies under consideration of the economic success factors time, costs and quality. Goal of the modelling approach - which is done in the first part of the project –should be the development of methods, which are able to integrate all building blocks of the facility (production, building, energy, logistics, management system) with one approach. This phase of BaMa started with a thorough system analysis and the definition of the methodology. In order to address these challenges, systematic approaches, as described by Thiede et al in “A systematic method for increasing the energy and resource efficiency in manufacturing companies” (Tiede et al, 2012) have been analysed. A modular approach was chosen, that segments a production facility into so called "cubes". In the first step the features of the cubes were defined. Cubes have in addition clearly defined interfaces and represent a certain physical behaviour that contributes to the energy balance of the overall system. Nevertheless all cubes should be built up with the same architecture.

One of the main goals of BaMa is to monitor and compute energy and resources consumption. For doing so, based on the cube related energy and resource flow analysis, the method should be able to generate a specific product-footprint for every product running through the “cube system”. The product footprint represents a products expenditures concerning cost, time, energy and the environmental impact such as resulting carbon emissions in the product life cycle phase within the factory.

Of course there are already comprehensive planning tools, such as (Bleicher et al, 2014), which also have been analysed. Regarding this analysis BaMa should also be implemented inside a customised toolchain. The toolchain (Balanced Manufacturing Control, BaMaC) allows energy efficient operation, design and refurbishment of production plants under competitive conditions, with regard to minimal energy and resource consumption. Tools to assist energy conscious steering of a plant during operation will be developed as suggested by K. Bunse et al in (Bunse et al, 2011). BaMaC will contain three core modules:

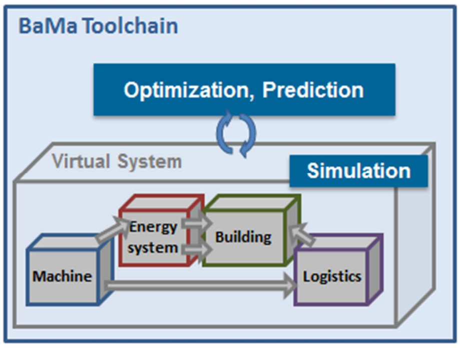


Figure 5.1: Future Modules of the BaMa Toolchain. The simulation approach has to fulfil various demands

The modules in detail will be able to support the three tasks: *Monitoring:* data on resources consumption will be aggregated and visualised, data can be implemented into simulation of cubes. *Prediction:* allows forecasting of overall energy demand of the plant based on the product-footprint and the production schedule. *Optimisation:* based on data and numerical simulation-models of the cubes, this part of the tool chain will improve the plant operation with regard to the optimisation targets energy, time, costs and quality.

By integrating the four main optimisation fields building, energy system, production, and logistics equipment BaMa will be applicable to a variety of industrial sectors. It will serve as a basis for a software tool chain which will be integrated into industrial automation systems, such as ERP or MES. The toolchain will introduce energy efficiency as a steering parameter into the control centre, thus enabling manufacturing companies to balance energy efficiency and competitiveness in their continuous operation strategies.

To satisfy the described demands of BaMA and BaMaC the cube concept needs to fulfil a variety of characteristics. The concept has to fit a variety of applications i.e.

it should be able to integrate all relevant building blocks of the facility (machines, energy system, logistics, …) with the same architecture. It is used as formal description of the real production plant and also as basis for models of the system. This modelling should be possible more or less “directly”, without much amount of work for translating. The cubes must have clearly defined features and interfaces and the system should be able to generate a specific product-footprint for every product running through the “cube system”. And finally of course implementation should be possible easy, fast and stable.

5.1.1 Motivation of BaMa - Footprinting

One of the most interesting demands – and main goal - in BaMa is the implementation of a comprehensive foot printing for industrial production plants. Industrial production accounts for 40% of the energy consumption of Europe, with an estimated potential for reduction of 30% to 65% (Bonneville et al, 2014). A common top-down approach to identify the environmental impact of products is to assess the Carbon Footprint of Products (CFP) on a one-year-basis. This procedure is important for raising awareness. However, for the purpose of optimizing plant operation it is not well suited, because the results can vary on a large scale due to the lack of transparency of different methods (Padgett et al, 2008), missing standardisation (Gaussin et al, 2008) and the lack of reliable data (Neugebauer et al, 2013. In addition the CFP fails to incorporate the diversity of different types of expenditure that go into the manufacturing of products.

In order to address these issues the BaMa bottom-up approach for aggregating a product footprint during the production phase of the product life cycle was proposed. This method allows for real-time evaluation of a batch or even single product using monitoring or simulation data. The definition of a significant footprint sets product success factors in context with its ecological impact. In particular energy, costs, carbon emission and time will be captured and visualised for the transformation process a product undergoes within the plant. Each part of the plant contributes to the product’s energy, cost or time consumption, as well as carbon emission, which accumulates the product footprint. The energy used by production machines, auxiliary infrastructure, logistics and the building is aggregated from the entry of the raw materials to the departure of the finished good. The integral footprint of all products produced in a year match the yearly carbon footprint of the plant exactly. Therefore comparability with conventional studies is achieved.

From this bottom-up approach different challenges arise. For example, the incorporation of standby-, setup- and ramp-up times, the energy consumption of the administration and the allocation of different products and by-products manufactured at a machine are some of the problems. The necessity to calculate mean values and dividing them between different products demands for a way to assess the degree of which each product is responsible for the generated footprint. One can easily see that measurement of data for this applications and modelling of such processes is challenging. Implementation would strongly benefit of a clear defined modelling concept and approved, straight forward methods. The cube approach, in which the system is described through black boxes (cubes) connected through inputs and outputs has to manage to map the complexity of a manufacturing facility in the necessary detail and breaking down the plant into its elements. The inputs and outputs of cubes can be material, energy or information flows. Energy flows carry a qualifier to determine the different expenditures, including carbon emission and monetary value. The products in the material flow accumulate the footprint by aggregating the cost, energy consumption, carbon emission and time inside the system boundary.

5.1.2 Requirements for Cubes

Based on the previous findings, a methodology for conducting a comprehensive system analysis of a production plant in preparation for the implementation of Balanced Manufacturing had to be developed. The methodology should be formulated at a generic level to ensure its usability in a variety of production facilities. As described the basic element of this system analysis consists of the so called cubes. The idea was that cubes constitute subparts of a system "production-plant" and have the following properties:

- defined boundaries,
- interfaces to other cubes,
- a certain physical behaviour that contributes to the energy balance of the system

and usually

- some degree of freedom to be influenced for optimisation.

To put it differently, the boundaries of sub systems in terms of energy-, material- and information flows had to be thoroughly defined to intersect the whole system into observable parts. The characteristics and attributes of cubes should be specified in a generic way in order to guarantee the applicability for all parts of the plant and for different kinds of productions. A cube could be a machine tool, a chiller, a baking oven, the production hall or a utility system. The definition of the cubes should allow implementing the described product-footprint evaluation, which sets the product success factors in context with its ecological footprint.

In particular the resources energy, costs and time will be captured and visualised for the transformation process a product undergoes within the plant. Each cube should contribute to the product's energy, cost or time consumption within the production plant which accumulates the product footprint. The product-footprint should be made up of a high number of originally independent data streams that are aggregated in a time-synchronised manner. So also methods for suitable data aggregation and fragmentation should be found and described.

So our approach leads us to the following process. (see Figure 5.2) . Analysis of the system (a variety of systems and their generalisation) leads us to the general "cube concept". This helps to formalise the real world and its control as well as future models. A formal model definition and implementation finalise the phase. In the first step we analyse general systems of production plants. As a matter of fact in BaMa a number of basic applications of real world system were taken to be analysed (e.g. production facilities of semiconductors, bakeries, metal processing industries, …). Based on these approaches several specific cubes are defined with a variety of needed features for input, output, system behaviour, system variables, changing processes and many more. An additional general analysis is done and a generic cube definition is formulated. This cube definition is one step before the formalisation of the modelling concept we will introduce. The modelling concept (formal model) will especially need to be able to handle continuous and discrete processes running through the "cube system". The last step is the implementation of simulation applications for BaMaC.

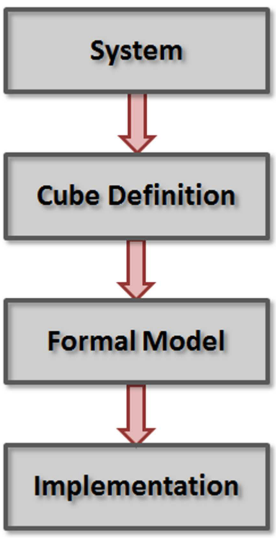


Figure 5.2: Overview Cube Concept

Most important at this stage was the demand, that the cube concept should be as generic as possible not including specific model restrictions at that time. For these demands ontologies seem to fit in some kind of way. For this reason - and as a next step - the basic idea of ontologies, as well as the motivation for using such ontological analysis in modelling and the role in the modelling processes should be described.

5.1.3 Ontologies in Modelling

After all analysis of the requirements for cubes showed that ontological analysis could be a promising approach. The project team thought at that time, that probably the project will not need the whole range of possibilities, but some aspects seemed promising. Ontologies have been an effective tool in modelling and simulation to help to address some aspects in complex modelling & simulation projects.

To understand principles of the ontological approach and to estimate benefits and motivations for using Ontologies in modelling we relied on the work of Benjamin et al "Using Ontologies for Simulation Modeling" (Benjamin et al, 2006). An ontology is an inventory of the kinds of entities that exist in a domain, their characteristic properties, and the relationships that can hold between them (Fishwick, 2004). In our case the domain is the part of the actual world, which is a production plant. Such a production plant has its own ontology, which we refer as a domain ontology with some sub domains. In a domain ontology, we define various kinds of objects (e.g., machines and tools), properties (e.g., being made of metal), and relations between kinds and their instances (e.g., part of).

In general we need to extract the nature of concepts and relations in any domain and representing this knowledge in a structured manner. An ontology and its building differs from traditional modelling activities (adding information and data to a formal system description) not only in depth but also in breadth of the information used. As Benjamin et al describe in (Benjamin et al, 2006): "Thus, an ontology development exercise will expand beyond asserting the mere existence of relations in a domain; the relations are "axiomatised" within an ontology (i.e., the behaviour of the relation is explicitly documented). Ontology development is motivated not so much by the search for knowledge for its own sake (as, ideally, in the natural and abstract sciences), but by the need to understand, design, engineer, and manage such systems effectively." For the cube concept, which should be used for various cube types within one model and as a basic library for future production plant models.

For defining ontologies different aspects are important as described in (Fishwick, 2004) especially determining the appropriate scope and granularity of ontologies and the use of ontologies as a basis for defining model repositories.

Inefficiency is often a problem in knowledge acquisition and management. Information that has been recorded before is captured again and modelling is done multiple times. Rather than having to identify information again and again in different applications, the idea of an ontology is to develop libraries " large revisable knowledge bases of structured, domain specific, ontological information in which can be put several uses for multiple application situations" (Benjamin, 2006).

The literature describes ontologies as important for modelling for a lot of reasons. Ontological analysis has been shown to be effective as a first step in the construction of robust knowledge based systems (Hobbs, 1987). Modelling and simulation applications can take advantage of such technologies. As a second point, ontologies help to develop standard, reusable application and domain reference models. This characteristic seemed to fit for integration of various production plant types. Last but not least ontologies are at the heart of software systems that facilitate knowledge sharing.

Motivation for Using Ontologies in Modelling

Basic motivations for using ontologies in modelling and simulation are that they are useful across the modelling and simulation lifecycle, particularly in the problem analysis and conceptual model design phases. They play a critical role in simulation integration and simulation composability and they are important in facilitating simulation model interoperability, composition and information exchange.

One of the key ideas is to allow the decomposition of the overall system model into smaller, more manageable components, and to distribute the model development effort among different organisations or functional groups (Benjamin, 2006). This is a perfect approach for the planned cube concept. Once the component simulation models have been developed, there is a need for mechanisms to assemble a simulation model of the entire target system in a manner that the "whole (system) = sum of its components."

An important challenge is modelling and simulation composability (from a set of independently developed components). "Composability is the capability to select and assemble simulation components in various combinations into simulation systems to satisfy specific user requirements" (Petty et al, 2003). Composability enables users to combine, recombine, and configure or reconfigure components in numerous ways to satisfy their diverse needs and requirements. There are two forms of composability: syntactic and semantic . Syntactic composability deals with the compatibility of implementation details such as parameter passing mechanisms, external data accesses, and timing mechanisms. Semantic composability, on the other hand, deals with the validity and usefulness of composed simulation models (Petty et al, 2003).

As a matter of fact these advantages of ontological analysis seemed to perfectly fit the needs of our cube concept and the formal modelling process afterwards. The process described in Figure 5.2 was perfectly set for application of the basic ideas of ontological analysis.

Role of Ontologies in the Modelling Process

Simulation models are often designed to address a set of modelling objectives or to answer a set of questions. An important first step in simulation modelling is to define the purpose of the model. This activity involves several related activities. On one hand the developer gets a "list" of not formalised problem symptoms. The domain experts often describe a problem in terms of a list of observed symptoms or areas of concern. The desire is to identify the cause of these symptoms and to suggest remedies. As described in chapter 1 one of the main objectives for the cube approach is to introduce the possibility of bottom up foot printing for production plants and to identify the origin of those symptoms. In addition often the domain experts specify the objectives of a project in terms of a specific question that needs to be answered, or, alternatively, specifies explicit goals to be met. For instance, in our example the manager of the production plant might ask the question "How can I optimise my production process?" or state a goal: e.g., "I need to reduce used energy by 20% on all my machines.". Using clearly defined objectives can help a lot in both cases to formalise and structure the described goals.

The purpose of the model also depends on constraints on possible solutions to the problem. The domain expert, based on past experience with similar situations, often suggests a variety of possible alternative solutions that must be explored. For example, a production plant manager who would like to increase production rate may, because of a budgetary constraint, be unwilling to invest in new machines, but may instead be able to hire additional labour. Ontologies will help facilitate the above tasks as well.

The advantages and also the justification of investing additional resources needed for following an ontological approach instead of doing only the work which is unconditional are on one hand providing a mechanism to interpret and understand the problem descriptions. Domain experts often use specialised terminology to describe symptoms and problems. Domain ontologies help with the unambiguous interpretation of the problem statements and in precisely conveying information about the problem to the simulation modeller. Cube can – in a reduced way – fulfil these characteristics. In addition harmonizing statements of objects that are described from multiple perspectives (often, this is a non-trivial task because of terminological differences and the lack of explicit descriptions of the semantics of different terms and concepts – see also [8]). Last but not least the ontological analysis unambiguously interprets limiting constraints that need to be addressed relative to accomplishing project goals.

All together the BaMa Cube concept will not fulfil all formal needs and demands of an ontology. As a matter of fact within BaMa the ontological approach was identified to support various needs of the modelling process. It helps in the process of getting “axiomatised” rules for the modelling of production plant sub systems. So the behaviour of the relations between subsystems is explicitly documented as well as the possibility how and what to “footprint”. Objects, properties and relations are clearly defined and are reproducible for every simulation project, that will be implemented with the cube concept. BaMa will not only generate “one model of one production plant” but will develop libraries and large revisable knowledge bases of structured, domain specific, ontological information in which can be put several uses for multiple application situations. In practice scope and granularity of the cubes can be defined clearly and can also be supervised. By using ontological analysis decomposition of the overall system model into smaller, more manageable components is done as well as distribution of the model development will be possible. The aim of composability enables future users of BaMa to combine, recombine, and configure or reconfigure components in numerous ways.

5.1.4 Cube Definition & Implementation

On basis of the above described ideas the generic term "cube" describes an encapsulated part of the observed overall system (domain). This is part of a methodological approach to address the high system complexity and heterogeneity by dividing the overall system from an energetic point of view into well-defined manageable modules (see Figure 3), which then allow a focused system analysis independent form the surrounding environment. Integrating different viewpoints and areas of engineering (machinery, energy system, building, and logistics) in a single system description can be interpreted as combining a number of ontological sub-domains and makes it necessary to establish a general specification of the cube properties and interfaces.

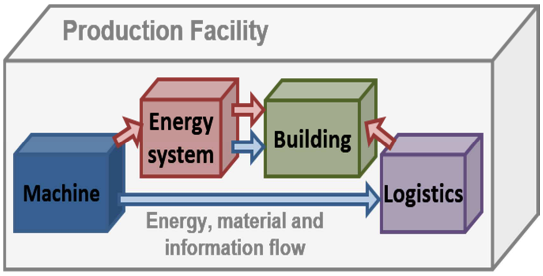


Figure 5.3: Production facility as interacting cubes.

The cubes consolidate all information and resource flows (energy, materials, etc.) within identical system boundaries, which not only promotes transparency during simultaneous analysis of energy and material flows, but the obtained modularity also increases flexibility for adaptation to specific environmental conditions.

Cubes have uniformly and consistently defined interfaces through which they interact with each other by exchanging energy, material and information flow, see Figure 5.4.

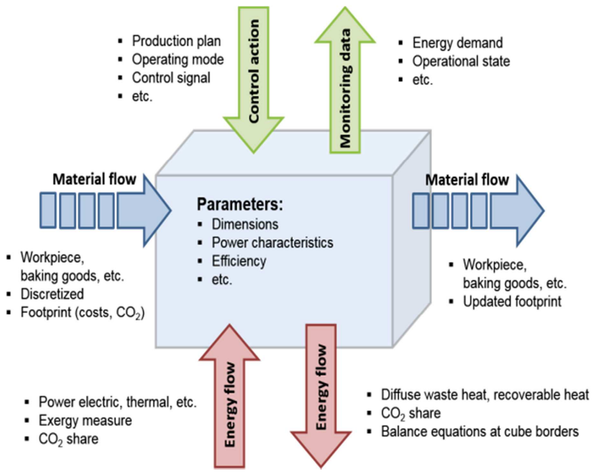


Figure 5.4: Generic cube interfaces with energy, material and information flows.

The material flow incorporates the immediate value stream (e.g. work piece, baking goods) and is described as discrete entities. All necessary energy flow (electrical, thermal, etc.) is represented as continuous variables together with their respective CO2 rates and is quantified inside the cube boundaries using balance equations. Information flow provides operating states and monitoring values for the higher-level control as well as control actions for the cube module

This modular cube description and specified interfaces then enables analysing and modelling the internal behaviour independent from its surroundings. For experimental analysis based on measurement data, cube interfaces can be equipped with measuring devices to detect incoming and outgoing flows. Also, experimental production cubes are being constructed which allow a more in-depth energy analysis and the inclusion of more detailed measurement information for developing data models and usage in simulation.

The modularisation of the observed overall system is not only used for developing simulation models for these systems. So the cubes have not only the "virtual simulation block" (so-called virtual cube, see Figure 5.5) in the form of a component in a simulation model, which we have to formalise later on but also the representation in the "real world" e.g. in the automation system of the production plant. The retained encapsulation and interaction via defined interfaces provides flexibility during internal modelling of the cubes (e.g. as mathematical models, data models, etc.) and for reusing implemented components in other models.

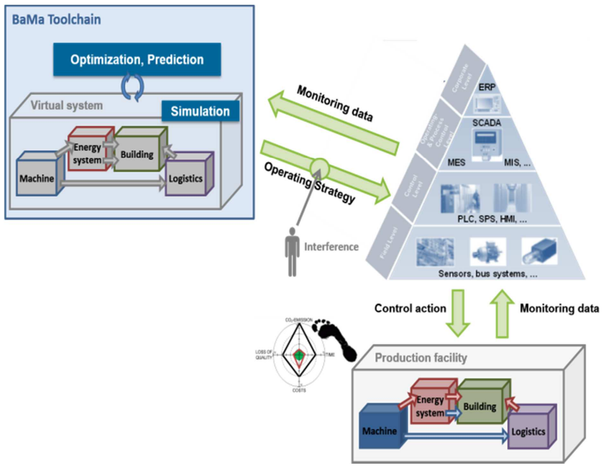


Figure 5.5: Architecture of the BaMa toolchain including the production facility in the "real world" and the a virtual representation of the observed system (simulation).

Figure 5.5 shows the relationship between real and virtual cubes in the simulation environment and the integration into the overall automation system architecture. The BaMa toolchain obtains measurement and status data from different levels of the automation system and on the other hand delivers prediction data and proposals for optimised operation strategies that can be adopted - with user interaction - in the real system. The generic interface and attributes definition of the cubes serves as a basis for specifying four cube categories (see Figure 5.6).

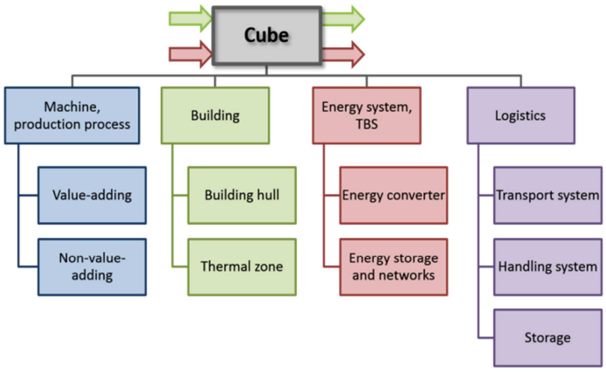


Figure 5.6: Categories and subcategories of cubes

Defining the cubes succeeded in the possibility to have reusable modules for representing machines and all other physical inventory within a production plant. Both discrete and continuous flows can pass through the system. The modules are on basis of one methodology (all cubes are children from a master cube, see Figure 5.6) and can so be implemented in the same way.

As a matter of fact while doing the cube concept, the modelling group of BaMa always had in mind how to formalise in the next step the model libraries on basis of the given features and interfaces, which was helpful in the next step.

Formalisation of Cubes

After the generic description of cubes the question of implementation arises. As far as described we combined various areas of production plants, where entities are able to pass from one area to the other. Still we need to be able to generate the planned foot printing. As described in the last chapter on the one hand, the modelling approach needs to provide solutions for hybrid systems, i.e. systems containing continuous as well as discrete parts. Of course there are many software tools which offer solutions for either continuous or discrete models but not for combined models. Still, there are a few commonly known simulation environments like Simulink or Modelica who allow the combination of discrete and continuous model parts. In the case of Simulink, for example, discrete SimEvents models can be combined with continuous models described by ordinary differential equations (ODEs) where the SimEvents scheduler and the ODE solver work in parallel and cooperate, which seems to work fine for very simple trials, but as soon as large or rather complex systems are implemented, the simulation can fail due to non-resolvable errors. Additionally, the execution of actions intended to take place at the same time an event occurs has to be defined by the user right before or right after the event in order to prevent unintentional results.

On the other hand in the BAMA project buildings as well as machines, building services and logistics have to be modelled and simulated on the whole in spite of their different requirements regarding modelling approaches and simulation techniques. As this is virtually impossible to realise in one tool alone, the most common way to face this task is to use cooperative simulation (co-simulation). There exist some co-simulation tools developed especially for systems containing buildings and machines, but most of them regard mainly thermal processes and perhaps energy consumption but disregard resources and do not support optimisation. Furthermore these tools in general gravely restrict the software used for partial models.

These problems were approached by taking the step between the generic description (Cube Definition) and the actual Implementation - using a simulation formalism (Formal Model) – see Figure 5.2. In 1976 Bernard Zeigler proposed in his book "Theory of Modeling and Simulation" (Zeigler, 1976) a classification of dynamic system-models into three basic types: Discrete Event -, Discrete Time – and Differential Equation – systems (DEV, DTS, DES). DEV are usually simulated using an event-scheduler, DTS are system models where changes of state-values are happening in equidistant instances of time and DES as purely continuous models, described with differential equations. Zeigler introduced system-specification-formalism for all three types (DEVS, DTSS and DESS) where DTSS is a subtype of DEVS.

Very important properties of the formalisms are their hierarchical nature and their closure under coupling which perfectly fits the cube features. That is, an atomic model of each formalism has inputs and outputs, which can be coupled with inputs and outputs of other atomic blocks or with the inputs and outputs of an overlying non-atomic model which inhabits these atomic models (hierarchical). The resulting overlying model now behaves exactly like an atomic model (closure under coupling) of the particular formalism and therefore again can be coupled with other atomic and non-atomic models. In the following part we assume the knowledge of atomic and coupled DEVs and atomic and coupled DESs (see Zeigler, 1976).

On basis of these atomic and coupled DEVS and DESS Zeigler introduced an additional formalism called DEV&DESS (Zeigler, 2000) standing for Discrete Event and Differential Equation System Specification. DEV&DESS is intended to describe so called hybrid system. In this context, hybrid system means a system consisting of both, a discrete and a continuous part, which is exactly what is needed for cubes.

An atomic DEV&DESS can be described by the following 11-tuple:

$$DEV\&DESS_{atomic} =< X^{discr}, X^{cont}, Y^{discr}, Y^{cont}, S, \delta_{ext}, C_{int}, \delta_{int}, \lambda^{discr}, f, \lambda^{cont} >$$

where

X^{discr}, Y^{discr}...set of possible discrete inputs and outputs

X^{cont}, Y^{cont}...set of possible continuous inputs and outputs

$S = S^{discr} \times S^{cont}$...set of possible states(=state space)

$Q = \{(s^{discr}, s^{cont}, e) | s^{discr} \in S^{discr}, s^{cont} \in S^{cont}, e \in \mathbb{R}_0^+\}$

$\delta_{ext} : Q \times X^{cont} \times X^{discr} \to S$...external state transition function

$\delta_{int} : Q \times X^{cont} \to S$...internal state transition function

$\lambda^{discr} : Q \times X^{cont} \to Y^{discr}$...discrete output function

$\lambda^{cont} : Q \times X^{cont} \to Y^{cont}$...continuous output function

$f : Q \times X^{cont} \to S^{cont}$...rate of change function ("right side" of an ODE)

$C_{int} : Q \times X^{cont} \to \{true, false\}$...state event condition function

The meaning of all sets and functions listed above follow classical definitions for DEVS and DESS with one exception: $Cint$. $Cint$ is a function of the actual state q and continuous input value $x^{cont}(t)$ and is responsible for triggering internal events, which then may cause a discrete output $x^{cont}(t) = \lambda^{discr}(q, x^{cont})$ and definitely results in the execution of δint.

Therefore, internal events in DEV&DESS are not exclusively dependable on time, as it is the case with DEVS, but may also be triggered because of the system state s reaching a certain threshold. Events of the latter type are called $state\ events$. Since the state transition functions δint and δext update the whole state, including its continuous part, they may lead to a discontinuous change in s^{cont}. Thus, as s^{cont} is the output of an integrator, this integrator needs to be reset, each time an external or internal event occurs.

The last distinguishing feature of the whole DEV&DESS from its components DEVS and DESS is the dependency of δint and λ^{discr} on the actual continuous input value. For DEV&DESS to be well defined, we need to fulfil both, the requirements for the DEVS part, and the requirements for the DESS part. Therefore for each possible input trajectory and initial state, during a finite interval of time only a finite number of events is allowed to happen. Furthermore again the function f has to meet the Lipschitz requirement

$$\| f(q,x) - f(q',x) \| < k \cdot \| q - q' \| \ \ \forall q,q' \in Q and x \in X$$

and the continuous input and output signals need to be bounded and piecewise continuous.

Since atomic DEVS can be coupled with each other and atomic DESS can be coupled with each other, also atomic DEV&DESS can be coupled. However there are some restriction concern- ing the coupling of continuous outputs with discrete inputs. A coupled DEV&DESS can be described by the following 7-tuple.

$$N =< X^{discr} \times X^{cont}, Y^{discr} \times Y^{cont}, D, \{M_d\}_{d \in D}, \{I_d\}_{d \in D \cup \{N\}}, \{Z_d\}_{d \in D \cup \{N\}}, Select >$$

where

X^{discr}, Y^{discr}...set of possible discrete inputs and outputs

X^{cont}, Y^{cont}...set of possible continuous inputs and outputs

D...set of involved ‘child DEV&DESS’ denominators

$\mathrm{M_d}$...child DEV&DESS of N for each $\mathrm{d} \in \mathrm{D}$

$\mathrm{I_d} \subset \mathrm{D} \cup \{\mathrm{N}\}$...influencer set of $\mathrm{d}, \mathrm{d} \notin \mathrm{I_d}$

$\mathrm{Z_d}$…interface map for d

Select: $2^{\mathrm{D} \cup \{\mathrm{N}\}} \rightarrow \mathrm{D} \cup \{\mathrm{N}\}$...tie breaking function

But there are some restrictions, concerning the coupling of discrete outputs with continuous inputs and vice versa. Therefore, the interface map Zd is divided into two component functions. One for the calculation of the discrete inputs of block d:

$$Z_d^{discr}: \underset{i \in I_d}{\times} YX_i \rightarrow XY_d^{discr}$$

and one for the calculation of the continuous inputs

$$Z_d^{cont}: \underset{i \in I_d}{\times} YX_i \rightarrow XY_d^{cont}$$

Then, we need to define how to interpret a connection from a discrete output to a continuous input and the other way round:

Discrete output signals, actually are only existent at the instance of time when they are produced. The rest of the time, the value of the output signal is the empty set $\emptyset$ or non existent. However, to enable connections between discrete outputs and continuous inputs, we define discrete outputs to be piecewise constant. So the value of a discrete output at a time between two output events is always the value of the last output event. Therefore, it is allowed to connect discrete outputs arbitrarily to continuous inputs. The other way round is not that easy, and it is necessary to apply restrictions. Thus, continuous outputs are only allowed to be connected to discrete inputs, if they are piecewise constant.

One could think of a connection from discrete to continuous being realized by putting an additional DEV&DESS block in between that receives the discrete output at its discrete input and forwards it to its continuous output. The other way around works as well.

As DEV&DESS sums up the functionality of both sides, the discrete and the continuous one, the modeller has to deal with the requirements of each formalism as well. On the one hand, the modeller needs to take care, not to produce algebraic loops and on the other hand he also needs to think of how to define the tie-breaking function select for the model to produce the desired behaviour. As Zeigler showed (Zeigler, 200), all three basic formalism, DEVS, DTSS (already included in DEVS) and DESS describe subclasses of the set of DEV&DESS-describable systems. Therefore DEV&DESS-describable is perfectly suited to formally describe and simulator-independently hybrid models of real systems. In our case - as a step in between - we used the cube formalism as organisational structuring of the modelling process using ontological analysis know how. Every cube has continuous inputs like various forms of energy, which are part of a continuous model, and many cubes, like machine cubes handling work pieces, have discrete inputs which are handled in a discrete system part of the machine model.

Since the DEV&DESS formalism does not specify solution methods, solution algorithms for the discrete part and differential equation solvers for the continuous part can be chosen at the point of implementation. In the case of cubes comprising purely continuous models, the DESS formalism can be applied and still linked with other cubes described by DEV&DESS or DEVS for plain discrete systems. Additionally, several atomic DEV&DESS can be embraced by another DEV&DESS called coupled DEV&DESS afterward for even better structuring; hence the DEV&DESS formalism also fulfils the hierarchy requirement, which represents an obligatory demand in the BAMA cube definition.

As every DEV&DESS, be it coupled or atomic, can be regarded as separate systems and each DEV&DESS represents one cube in which the balance equations consider everything within the cube's borders, which are per definition balance borders, closure regarding balance equations can also be ensured as long as the generic description of the cube can guarantee it.

DEVS is a very general formalism. As a result, it can be shown, that a lot of other discrete-event-formalism, as for example Event-Graphs, State charts, Petri-Nets and even Cellular Automata describe subclasses of the set of all systems describable by DEVS. That's why Zeigler proposes the so called DEVS-Bus as common interface for multi-formalism simulation. For implementation and formalisation this keeps the possibility of a "general approach" for integrating domain experts knowledge in future approaches and involve possible additional model concepts (e.g. additional cubes shall be described in one of the ways mentioned above).

Implementation

Last but not least, since digital computers only are able to work in a discrete way, discretisation is necessary for each DEVS and DESS-part of a DEV&DESS to be able to be simulated on a digital computer. For pure DESS-models, usually ODE-solver-algorithms are used, to numerically solve the differential equations, i.e. to simulate the DESS model. Therefore, the DESS model in combination with the used ODE-solver constitutes a DEVS model, approximating the DESS model. This resulting DEVS model, as each DEVS model, can then be simulated error-free on a digital computer, apart from the error due to the finite representation of real numbers.

But due to the fact that the DEV&DESS formalism is, as its name implies, just a formalism, it is independent from the implementation software. This is very important for the BAMA project since a lot of participating industry partners already use certain automation software which is intended to be able to communicate with the simulation software and every developing partner has preferred simulation tools or limited licenses.

The DEV&DESS formalism does not restrict the possibilities for the cube interfaces. In the cube definition described briefly above it has been defined that input and output signals can be arrays and may represent physical values which carry a unit or other attributes ensuring consistency. This is possible with the DEV&DESS formalism since the only specification for inputs or outputs to a DEV&DESS is that there is a set of discrete and/or a set of continuous inputs and outputs. Hence the demands on cube interfaces can be met by the DEV&DESS formalism. Finally taking a deeper look at ontological analysis was worth doing, even if BaMa did not implement its own ontology. Defining and implementing the process as described below (see Figure 5.7) was one of the keys to successfully implement the cube methodology in the first phase of BaMa.

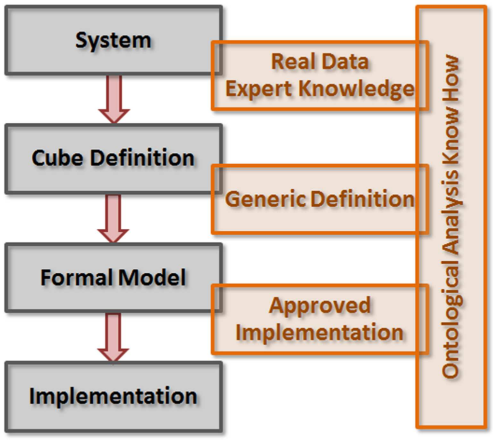


Figure 5.7: System Analysis and Modelling uses Ontological Analysis Knowhow for reusable, quality assured results.

At the actual point of BaMa the definition of the DEV&DESS formalism is finalised. As a matter of fact there is still a link missing to get to the implementation itself, but on the one hand there exist several tools implementing the DEV&DESS formalism with a certain approach like PowerDEVS using QSS for the discretisation of the DESS parts and thus transforming DEV&DESS into DEVS only, QSS-Solver with the Micro-Modelica language, M/CD++, or a Simulink library for DEV&DESS developed at the Hochschule Wismar or DEVS-only tools like DEVS-Suite, CD++ and JDEVS; on the other hand in the course of the BAMA project several typical scenarios have already been formalised with the DEV&DESS formalism and implemented PowerDEVS for test purposes, so it is warranted that this formalism can actually be used as a bridge from the BAMA cube definition to the BAMA implementation.

5.2 Basic Idea of the Simulation Pipeline

The basic concept for an extended simulation pipeline was invented for the area of Health Technology Assessment (HTA) (see Popper et al, 2012a; Popper et al, 2013). HTA provides information for decision-makers in the health care system and the general population and is a very well standardised scientific process itself. Therefore it is optimal regarding, development of an "accompanying" simulation process. The section is based on (Popper et al, 2012b).

With IFEDH (**I**nnovative **F**ramework for **E**vidence-based **D**ecision support in **H**ealthcare) the idea was to design a new strategy for the integration of modelling and simulation into the HTA process within limited resources whilst staying open to emerging new technologies.

Dynamic and static modelling is becoming more and more essential to the HTA process. Simulation can help decision-makers contrast and assess various technologies that compare different goal functions on a basis of evidence. This can only be fully achieved via a reliable and reproducible process of simulation modelling and computing.

5.2.1 Overview IFEDH – an Innovative Framework

The fundamental framework that was developed, which links the fields that are most important to providing a basis for decision-making, will be outlined in detail. This includes the formulation of PICO questions, data acquisition and evaluation, model development and results interpretation. The Innovative Framework for Evidence based Decision making in Healthcare was funded by the COIN – Cooperation and Networks program of the Austrian Research Promotion Agency (FFG, project number: 827347).), the national funding institution for applied research and development in Austria.

With an interdisciplinary group of experts in the field of HTA the tasks was to integrate statistics, modelling, visualization and database analysis through the entire decision support process. Application areas were infectious disease simulation and vaccination questions, as described above. However, the methods derived thus are also directly applicable for all other questions in HTA. Beyond tackling the complexity of guiding and controlling the coupling of different scientific domains in order to put into practice a joint overall approach in model-based HTA, new approaches had to be developed and implemented in all of the fields involved.

Growing demand for faster decision support necessitates the advance development of parameter sources and modular reusable model parts. However, the modelling process and the design of adequate modelling methods constitute only one (albeit core) part of the project. Beyond this, model and parameters have to be validated and the system that has been developed and implemented needs to be verified. The interdisciplinary set-up for data quality assessments and the outcome visualization and interpretation ensures that the project meets the required quality standards and is sufficiently accepted by policymakers.

The project's scientific partners were the Main Association of Austrian Social Security Institutions, the Ludwig Boltzmann Institute for Health Technology Assessment, the Vienna University of Technology (VUT) and the VRVis Centre for Virtual Reality and Vizualisation; its company partners are dwh Simulation Services, E.I.S. Ltd. Florian Endel and FWD GmbH. UMIT - Private University of

Health Sciences, Medical Informatics and Technology-GmbH acts as an additional contributor.

The first step of the project entailed the analysis of model and structural know-how and parallel collection of information on the state of the art of modelling in HTA in Austria. Based on this information, the project participants specified model structure requirements as well as a standard for the documentation of simulation outputs. This was the second step. In the third step, the network embarked on one of its core tasks: the development of adequate/reusable modelling structures and modelling methods. An evaluation table was compiled for this purpose, showing methods in use as well as modelling and simulation strategies from other domains that may be employable in HTA.

In addition, modular model parts were developed and tested for their reusability. The analysis of data sources relevant to each module as well as the realization of usability tables and interface descriptions concluded this task, ensuring high flexibility and reusability. Based on this outcome, exploratory research was conducted on the following topics:

- different modelling techniques of infectious diseases (Zauner, Popper & Breitenecker, 2010)),
- herd immunity effects in population groups using agent-based modelling methods (Miksch et al, 2010) and
- IFEDH member research on serotype behaviour modelling for infectious diseases and vaccination strategies (Zauner et al, 2010)

Recommendations for good practice were developed on the basis of this research.

A "good practice" manual was developed in accordance with the evaluation and integration of classical HTA methods, their development for data preparation and analysis on Austrian reimbursement data. The elaboration of standardized visualization concepts for

1. model parameters,
2. model structures and
3. the results,

together with research on scenario set-up and sensitivity analysis work-flow were integrated and tested for practical use by implementing three real world HTA questions. Examples were taken from the fields of, firstly, influenza transmission, secondly, HPV vaccination and its influence on cervix carcinoma and, thirdly, an instance of the evaluation of abdominal aortic aneurysm (AAA) screening.

The IFEDH research project began with an evaluation of the status quo, which consisted of the following tasks:

- Documentation of standards in modelling and simulation in the field of health technology and health system evaluation
- Documentation of standards in HTA: this documentation describes the standard process in vaccination program evaluation as well as the methods used and their limitations. Expert opinions and a structured questionnaire are used in order to establish the state of the art in Austria and neighbouring countries.
- Documentation on problems that have been identified in the representation of solution pathways: This documentation lists open questions that had come up in earlier projects conducted by project partners using modelling and simulation for evaluation of vaccination scopes. The solution strategies that were applied and the discussion about a general application of the given strategies are documented for each problem.

This first step provided the basis for the formulation and realization of the second step, the definition of demand profiles for modelling and simulation in HTA.

The definition of a mutual language is key to the success of this interdisciplinary project, bringing together, as it does, partners from different fields who have to work together and understand each other. Both the development process and the resultant service are dependent on the ability to successfully to so. Hence, a glossary was compiled on the basis of international definitions and formulations used by the individual project partners. To guarantee the glossary's constant currency, this document is defined as an open document type that is continually expanded by the partners throughout the entire project period. Inconclusive or "parallel" formulations are discussed by project participants from different domains and the consensus decisions are binding for all partners.

The compilation of requirements for the model structure and documentation of simulation outputs mark the final step of the first project phase. The essentials are determined in order to ensure an efficient modelling process in which the models subsequently do not have to be changed too frequently. The processes of selecting a question for decision-making (prioritisation) and of evaluating the findings within a broader political context (appraisal) are not covered in detail. These aspects are, particularly in Austria, largely influenced by political decisions. However, again we address the issue of how to generate a reasonable question for the modelling process, in this domain on basis of the PICO question.

5.2.2 The Research Question & Resulting Data Analysis

Working on a relevant problem in HTA usually requires first of all a clarification of the potential decisions, the definition of the population/ condition in question, the intervention, the comparator and the outcomes of interest. This is the format of the PICO (**P**opulation, **I**ntervention, **C**ontrol, **O**utcome,) question, with was mentioned in the process development earlier. In this phase of scoping, the question has to be worded as precisely as possible, while at the same time the feasibility and necessity of modelling have to be discussed. Knowledge of the health care system is essential to understanding the various paths the HTA process can take. The political decision-making process can be visualized as shown in Figure 5.8.

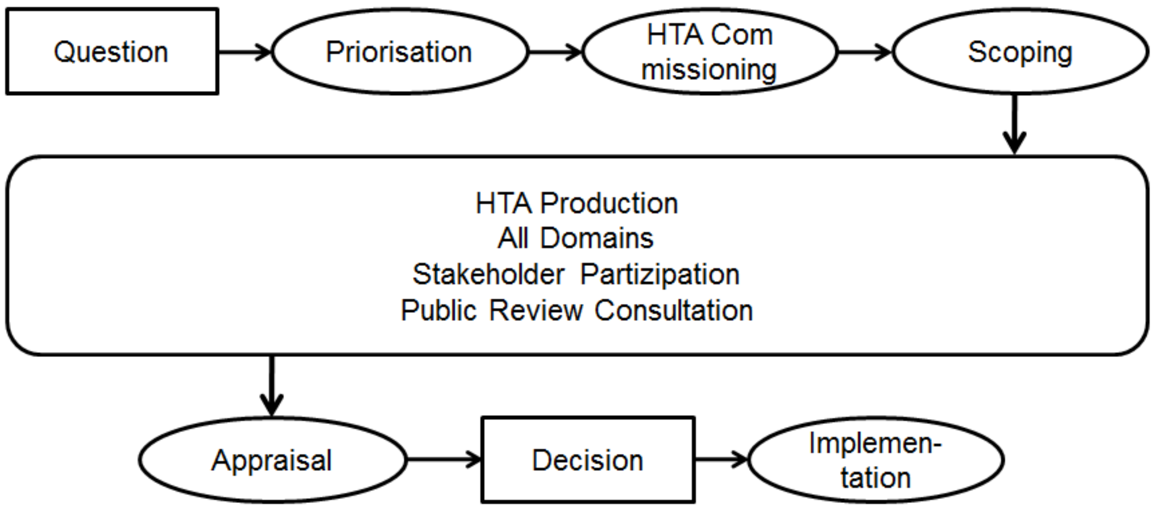


Figure 5.8: Decision-Making Process The figure shows the political sphere, the administrative aspect, the core working area of HTA institutes, the appraisal and the health system

Having arrived at the PICO question, there follows the identification of which part of the HTA process can be supported by modelling and simulation. It had to be decided which research questions can be answered using models and what steps have to be taken in order to be able to do so. These decisions were undertaken by a steering group covering the various aspects that come into play. The PICO question itself is always the starting point. Based on this, the problem's data and structure have to be analysed. The modelling technique is developed and decided on in an iterative process (still within the steering group). A special documentation process is followed in order to guarantee that the process can be handled as planned and quality management is kept up.

By the end of this process, an exact definition of "not model-based" HTA questions and of the questions that can be handled with methods of modelling and simulation had been arrived at. The modelling process was started on the basis of these questions; the method and the exact specifications of the model were decided on. Finally, the complete parameter and data set was defined. This set is necessary for the implementation of the basic simulation as well as for all comparative scenarios. The decisions were then communicated throughout the interdisciplinary team.

There followed the process of data acquisition, while reliable and reproducible documentation had to be completed simultaneously. IFEDH has developed and described a focused procedure (on the basis of the EUnetHTA project and the HTA Core Model) for the description of the process and the status of used data. A web tool – the HTA manager – is used for the documentation of the source, status and manipulation of data. The HTA manager allows for permanent documentation of all necessary data for all simulation runs (i.e., the basic simulation, such as the *status quo* of a given therapy, as well as all possible scenarios, like a new vaccine or new regulatory requirements). This is made possible by a three step documentation process. The first step is to document the sources for all data sets. There are three different categories of used data:

- CKAN data (using one of the world's leading open-source data portal platforms, http://ckan.org),
- other open data sets, and
- private or confidential data, e.g., insurance association data.

The second step documents modifications made to any of the data sets. These adaptions may include, e.g., SQL requests, filters or any other modifications of the given raw data sets. Step three consists of the download or storage of the used data set for (1) all parameters, (2) all simulation runs and scenarios into the HTA manager. This third step is the most important part of the documentation, as the given data and a full documentation of the model and implementation allows for the reproduction of the simulation runs for the basic system and all its scenarios at any time and from any place.

This capability is one of the IFEDH project's main goals, raising, as it does, the credibility of modelling and simulation within the HTA community. Another methodological goal of IFEDH had been the development of standards and methods for data preparation and data analysis. Requirements on data and their statistical preparations were provided for the generated model structure definition. A special emphasis was placed on the necessary quality and the granularity (i.e., how detailed the data provided had to be). Again, these steps were completed by interdisciplinary groups benefiting from results that are widely comprehensible and applicable.

A data quality assessment concept was designed following on from the identification of the granularity and the data sources. This concept explains the data quality assessment that has to be performed using health data, including theoretical principles, health data characteristics and implementation information. The following figure (see figure 5.9) shows the connection and interaction of modelling & simulation, parameterization and data quality assessment. The influence of the quality of data input, parameter estimation and modelling structure (simplifications, unsure assumptions ...) was discussed in an interdisciplinary context. In an early project phase, the goal was the identification of problems in parameterization and the sensitivity of diffuse parameters.

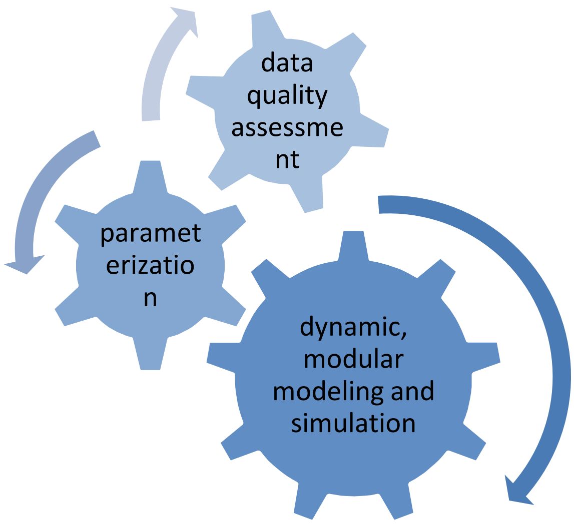


Figure 5.9: The connection between dynamic modular models, their parameterization and the data quality assessment is shown

The importance on the parameterization based on model structure and time intervals simulated is obvious. Furthermore, data quality assessment affects the parameterization (availability of data sources, reliability of parameters and range of confidence interval). Information about missing data quality or even the lack of data results are needed for changes made to the model structure or in additional HTA literature research as well as when searching for alternative parameterization attempts. The model certainly has to adequately match real-life conditions. Therefore, the interdisciplinary group had to reach a consensus in the early project stage. Changes made during a later phase generally cause a tremendous additional workload and may cause problems where changes in the model structure have to be justified to decision-makers.

An important aspect within IFEDH was the usage of routine data in HTA, as gathering data tends to be a costly and time-consuming task. During the course of the IFEDH research project, different methods for using routine data on models in HTA were discussed, improved on and developed. The project aimed to connect the rich data set from Austria's inpatient sector that lacks patient identifiers with the somewhat personalized but sparse records from the outpatient sector provided by different social security institutions. A detailed description of the setup and usage of the results was presented at the SHIP Conference 2011 in St. Andrews (http://www.scotship.ac.uk/conference-2011) and the International Data Linkage Conference 2012 in Perth (http://www.datalinkage2012.com.au/).

Documentation of prior processing and information of the provided data were not fully available; further technical and contextual challenges arose from questionable data quality and possible duplicates. Following preparatory steps including prepossessing and data quality assessment, a deterministic record linkage approach was developed using a combination of the open and freely available statistical environment R and PostgreSQL database. Based on dynamically created SQL statements and extensive logging, the linkage process can easily be enhanced as soon as new knowledge is gained about the input data.

The resulting linked data set provides high quality information that is immediately available. Furthermore, the deterministic linkage process can be examined and understood by its users. This makes it easy to identify linkage and data errors; feedback can be used to enhance the overall result. These experiences can provide a basis for more advanced linkage methods and further improvements.

After a long and challenging development from the first data import to a functioning data collection, adequate information can now be employed in different projects with high user confidence and at low cost.

5.2.3 Modelling & Visualisation

One of the network's core tasks is the development of adequate/reusable modelling structures and modelling methods. Modular model parts were developed and tested for their reusability. The analysis of data sources for each module as well as the realization of usability tables and interface descriptions completed this task, ensuring high flexibility and re-usability. One of the main advantages of this structure is the growing interdisciplinary knowledge base due to organized feedback.

Recommendation for new questions were developed on the basis of exploratory research on different modelling techniques for infectious diseases (Zauner, Popper & Breitenecker, 2010)), research on herd immunity effects in population groups using individual-based modelling methods (Miksch et al, 2010)) and research conducted by IFEDH members on serotype behaviour modelling for infectious diseases and vaccination strategies (Zauner et al, 2010).

Once again, the use of modelling and simulation in HTA was discussed in order to explain the decision of which technical approach to use. Furthermore, the following questions were identified:

- Formulation of the problem: What are the questions that shall be answered?
- Concept of the model: Which values are important, which of these describe the states of the model, which are parameters, which values influence the model in general? How are the values related?
- Is the model concept useful: Is there enough knowledge and data available to implement the model? Can the proposed questions be answered using the model if the model assumptions are true?
- Can the model be validated?

Next to the identification of useable modelling methods for answering HTA questions, the description also includes the classification of different viewpoints. This classification can be helpful when HTA experts are integrated into the process, even if they are not specialists in modelling and simulation. The classifications chosen are

- Black-box versus white-box modelling
- Top-down and bottom-up approaches
- Classification representing time

HTA and data experts are particularly aided in their understanding of the performance potential of modelling and simulation by interpretations of the differences between top-down and bottom-up modelling techniques and an explanation of processing of time. Beyond that, the discussion stimulates communication on usable formats for data provision. This stimulation, combined with an extra task and proof of concept examples, raises the quality of the service developed by the IFEDH partners. Where the methods defined are restricted and no other method from the project's first stage can be employed, it has to be considered how different methods may be combined. The starting point was the definition of the problem/the HTA question. The crux of this system is the fact that the data structure analysis is performed before the modelling method is chosen. The modelling process is nevertheless performed iteratively. The hybrid decomposition as well as the comparison of different methods and modular use of pre-developed tasks is part of the IFEDH research project's newly developed concept.

A particular focus was placed on the development of reusable parts of the model and in particular on their theoretical background. Their advantages and disadvantages, restrictions and potential applications in the field of evaluation of vaccination strategy were discussed. A general framework (see figure 5.10) was

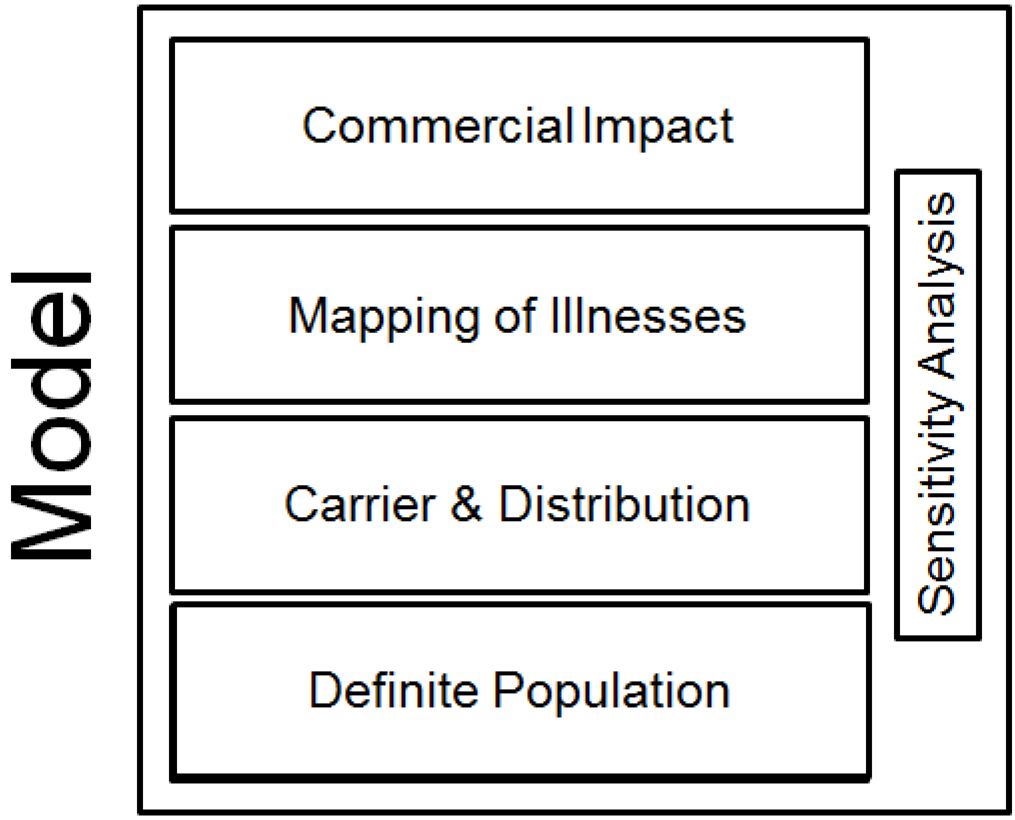


Figure 5.10: Example for splitting a cost effectiveness analysis HTA question into modular parts and a sensitivity analysis. The population modelling module is defined as reusable, the contact model can be exchanged due to well defined input/output structures

developed and tested using pre-defined proof of the concept examples that were processed together by the different partners in IFEDH.

The fundamental question on the connection of the model and the method of feeding the parameters into the framework is made apparent. A discussion on the following methods ensures the reliability and the quality of the data sets used:

- sensitivity analysis – using this method, the HTA and modelling experts gain knowledge on the overall influence of parameters of interest,
- parameterization and calibration: Calibration is a systematic adjustment of model parameters that are either unknown or uncertain (Taylor,

2007). The strategy is to adjust these questioned parameters in such a way that the model results sufficiently match the data provided.
- verification,
- validation, and, finally,
- simulation experiments and scenarios that provide results.

Calibration is a process of setting parameters, running the model, assessing the results, adjusting the parameters based on the results and running the model again. This procedure is performed until the results are satisfying. There are two types of situations that require calibration of a model (Taylor, 2007):

- When data are inadequate or missing, in order to estimate all model inputs.
- When the validity of a model is being questioned.

The development of hybrid modelling methods and modular model classification in the field of communicable diseases and especially for vaccination questions in HTA, combined with the compilation of a list of the main working tasks for parameterization brought this central task of the IFEDH project to a close.

The development of standardized visualization methods and representation of results was integrated into the project in order to generate additional insight into the model structure, to help explain the calculated results and also to provide a powerful graphical tool for parameterization.

The workload was split into several tasks, within which the analysis of state of the art methods in HTA was one of the first. Additionally, in order to encourage thinking outside the box, adequate visualization methods from other areas were detected and analysed and rated regarding their potential use in modelling questions for HTA. This rating was directed by the visualization experts together with the modelling group and classical HTA experts.

The other tasks were mainly based on the data basis for visualization. A guideline for the visualization of a generally evaluable data basis for vaccination program evaluation and the explorative analysis and visual inquiry of data quality was developed. Methods from other application areas were introduced into HTA for results visualization. To name only one, parallel sets were integrated as an interactive visualization approach for analysing Markov models, since common methods to visualize Markov states over time (e.g., Markov-cycle trees or state probability graphs) do not scale well to many cycles and are limited in their perception of proportions. These limits were overcome with an investigation into new visualization methods of Markov models and their results, inspired by the

"Parallel Coordinates". An interactive technique called Parallel Sets was developed for visualizing multidimensional categorical data. (Urach et al, 2012) The visualization lays out axes in parallel, where each axis represents one categorical dimension. Within each axis, boxes represent the categories which are scaled according to the respective frequencies. Applied to Markov models, the categorical dimensions correspond to the various cycles. Joint probabilities of categories from adjacent axes are shown as parallelograms connecting the respective categories. The parallelograms can be interpreted as the number of patients transiting from one state to another. Depending on the purpose, the colour of the parallelograms may indicate the categories of a chosen cycle or may refer to additional attributes of the patients, such as age or sex. (see Figure 5.11)

State probability and survival curves merely show specific aggregates of the data, while classic Markov trace visualizations with, e.g., bubble diagrams do not visualize data in such a way that it would facilitate a detection of proportions and trends. Applying Parallel Sets to analyse Markov models provides an interactive visualization technique where changing the reference Markov cycle is as easy as highlighting particular dimensions, thus enabling the exploration of the progress of patient cohorts with certain characteristics through the model. Model development always requires thorough analysis of its structure, behaviour and results.

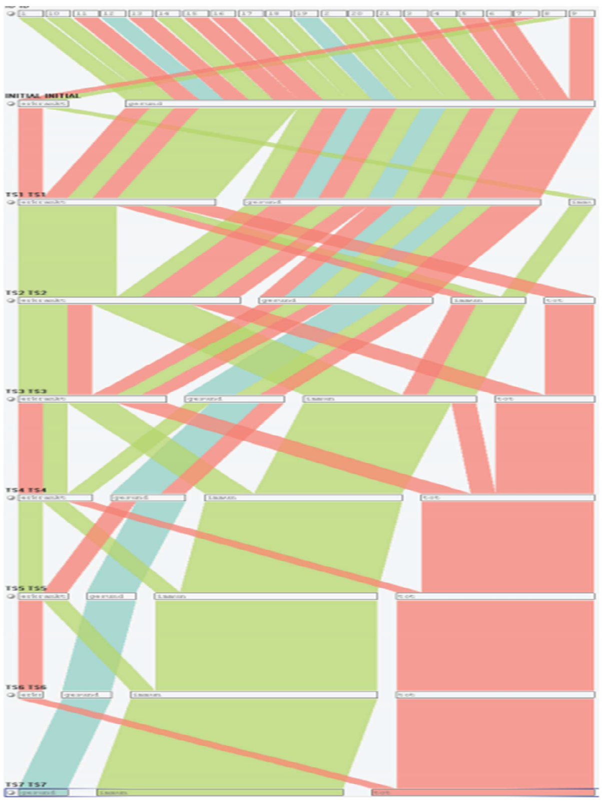


Figure 5.11: Parallel Sets enable an intuitive and efficient visualization technique for presentation purposes as well as exploratory analysis

The research project description presented shows how different expert domains can be united into creating a joint approach in model-based HTA of infectious diseases and vaccination strategy evaluation. A predefined work plan, parameter sources and modular reusable model parts are developed in response to a demand for faster decision support in an era of globalized human interaction and hence transmission of infectious diseases across borders and continents.

The theoretical research conducted in the field of statistical methods, testing of adequate visualization methods and data quality assessment tools as well as the development of a content management tool for the process guarantee that time restrictions and quality requirements can be adhered to. The modern modelling methods that were developed and the interdisciplinary process that was established deal with the questions arising in HTA in particular with regard to infectious diseases and the evaluation of vaccination strategies. The knowledge developed thus and the hierarchically structured framework aid the realization of an adequate system of decision support for model based HTA questions. A closer look at Austrian data and the Austrian healthcare system provides a fast implementation process for real world tasks.

5.2.4 The DEXHELPP Project

The IFEDH Pipeline was developed between 2009 and 2011. Based on the promising results of the project the next step was to be taken. According to the still developing needs of the domain "Health System" as described in section 1.1.2 and based on the results presented in this work, the author and Felix Breitenecker developed together with a consortium of partners from science, decision makers and industry the project DEXHELPP.

DEXHELPP started in 2014 and based on the research implemented the concept, which was international evaluated, was designed to fulfil the goals described in section 1.3.2. The difference an d additional benefit to the IFEDH project can be summarized that DEXHELPP focusses not only on health technology assessment, but the whole domain of Health System Research. Based on the findings of IFEDH and the modelling & simulation theory developed by Felix Breitenecker's group and on initiative and coordination of the author the concept was extended in all steps of the simulation pipeline. Beginning from improvements in data analysis, visual analysis and process quality assessment, especially the development of sustainable concepts is in the focus of DEXHELPP. To give an example, an important part is to develop a permanent population model of Austrian population matches with the Epidemiology. In this project, the burden of disease for Austria will be described and offered for all research groups interested to produce comparable and sustainable results. All models developed should be modular, so that once developed, special concepts for e.g. the spread of epidemics can be re used as good as possible. A research server will be implemented, where the presented simulation pipeline and processes will be physically integrated to prove the presented concepts of this thesis.

The concept and first results of DEXHELPP, where presented at Mathmod 2015 conference in the mini symposium “Interdisciplinary Data based Modelling and Simulation in Health Systems Research – Theoretical Development and Real World Applications”.

6 Summary & Outlook

The thesis is a summary of several years of research in the area of applied modelling & simulation of complex systems. The work presents theoretical concepts to give an idea how model comparison can be improved and summarises developed methods and applications. This is done on basis of knowledge of the practical problems and questions, which arise in interdisciplinary, medium sized research projects in this area. Motivations, tasks and resulting goals for modelling complex systems are presented in chapter 1.

Main goals of this work are **to improve both, the possibilities to compare modelling approaches and to improve the possibilities to combine them**. Better combining potential leads us to the question when and how to combine and how to switch between models. This is one of the important improvements of the introduced modelling circle.

In this context in chapter 2 different comparisons of methods are outlined. Starting from the simple alternative modelling of diffusion based equations with a cellular automaton, the comparative modelling of a SIR epidemic is presented. Transfer of parameters between comparable models is shown. A formal model is introduced to be positioned "above" (or before) the modelling with special formal concepts. This shows the theoretical potential of comparing different modelling approaches, which is later described for an applied research project.

In chapter 3 the general concept how to develop optimal research questions for modelling & simulation projects is in the focus and later underlined with various examples in different complex systems. The need for - and limitations of - formalisation of modelling concepts is presented. These are crucial for comparison of models. Examples for formalisation of cellular automatons, analysis of agent based models and limitations of homogenous modelling concepts are presented.

Based on these findings, questions of coupling of models to solve complex systems, which are divided in heterogonous subsystems, are discussed and various coupling methods are introduced. Resulting implementation tasks are outlined on the example of co-simulation. Last but not least an example for a concept to transfer a modelling approach (DAEs) to another domain (Health System Research), to handle rising complexity with new modelling methods, is defined.

In chapter 4 the question of reproducibility is addressed. The general process for modelling & simulation processes is presented, with a special focus on validation and verification of agent based models (as there are no sufficient theories so far) and the potential of visualisation within modelling & simulation theory.

Additional some examples for **resulting approaches** for specific aspects like the concept of cross model validation and the concept of falsification as reasonable research questions are summarised. Cross model validation helps to improve the ability to separate system immanent and model immanent behaviour and improves the opportunity for validating models of complex systems and processes, where real data and system behaviour is not applicable for classical validation.

Last but not least in chapter 5 **solutions for examples in medium scaled research projects** in modelling and simulation from the areas complex functional infrastructure and complex decision making are presented. For complex production facilities a modelling technique is introduced, containing a number of abstraction levels. This approach helps to standardise the formalisation process for various sub domains on the one hand, and still allows a flexible, modular and reproducible implementation of the simulations. Second, the concept of a reproducible simulation pipeline in health system research is presented, from data acquisition up to the decision support.

Future Work

The thesis can only give an overview of the wide range of problems addressed. The intention was to present both, a good overview of the work which was done on one side, and on the other side a profound selection of examples for implemented solutions both in modelling & simulation theory as well as in applications.

Still a lot of research has to be done. One problematic aspect is how to deal with the comparison of (1) modelling within one method in contrary to (2) develop multi method models, which have to be coupled. The first can be tackled with the outlined, improved formal extension of modelling approaches, the latter with presented concepts of coupling. But the question is, how complexity of systems can be measured to find the optimal concept to use. At the moment the trade-off is only described very vaguely. Complexity of a system should be measured via the effort of the approaches to be developed. A concept within the modelling process has to be outlined and worked out. In addition a lot of formal questions arose of the outlined approaches in this work.

Only as one of many examples for rising questions, the point of fixed number of agents in formalised agent based models can be mentioned. Complex systems, which have an evolutionary behaviour, need the possibility of generating and destroying agents.

Additional the general question how formalisation and parametrisation of systems will be done in future (based on big data or based on system knowledge, and how these approaches can be joined) is a crucial question in the area of modelling & simulation of complex systems.

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8 List of Figures

9 Curriculum Vitae

Name	Nikolas Popper
Citizenship	Austrian
Date of birth	27.02.1974
Address	Schottenfeldgasse 84/14, 1070 Vienna, Austria

Appointments

since 2014	**Coordinator COMET K-Project DEXHELPP** ("Decision Support for Health Policy and Planning: Methods, Models and Technologies based on Existing Health Care Data")
since 2013	**TU Wien, Project Assistant, Coordinator AMSDM-group** ("Applied Modelling and Decision Making")
since 2010	**CEO "dwh GmbH"** simulation services & technical solutions, INITS funded
2007-2008	**Parental Leave**
2004-2014	**CEO Landsiedl, Popper OG** (film production "die drahtwarenhandlung")
1999-2003	**ORF** "Bildung & Zeitgeschehen" (FI2), Position: science editor

Higher education

2009-2015	**Doctoral Programme in Technical Sciences** at TU Wien
2000	University of Idaho
1997	Universitat Politècnica de Catalunya
1993-2001	**Master in Technical Mathematics** at TU Wien (Diplomstudium technische Mathematik),

Selected Funded Projects Initiated

2013-2015	**Modyplan,** funded by ZIT, development of simulation tools for resources planning in health care, in cooperation with two institutes at TU Vienna Position: project coordinator
2010-2012	**IFEDH (Innovative Framework for Evidence-based Decisionmaking)**, funded by FFG, 10 project partners from science, public health, economy, Position: project manager
2010-2012	**MoreSpace**, funded by ZIT, in cooperation with two institutes at TU Wien, Position: project manager
2011-2012	**AMSDM**, funded by ZIT, building cooperative networks for modeling & simulation with TU Wien, Position: project manager

Other relevant activities

Co-Organization of MATHMOD 2009, 2012 (Vienna International Conference on Mathematical Modelling)

SNE "Simulation Notes Europe"-Journal: **Member of the Special Issue Editorial Board**

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