

# Minimization of Stochastic Dynamical Systems

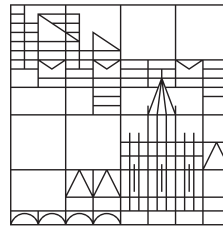
A Comparison of Models & Methods

## M.Sc. Project Report

by

Fabian Klopfer

Universität  
Konstanz



Faculty of Sciences

Department of Computer and Information Science

Modelling of Complex Self-Organizing Systems Group

**Supervisor:** Dr. Stefano Tognazzi  
**Professor:** Prof. Dr. Tatjana Petrov

Konstanz, 2020

# Contents

<b>1. Introduction</b>	<b>3</b>
<b>2. Models</b>	<b>4</b>
2.1. Automata . . . . .	4
2.2. Differential Equations . . . . .	4
2.2.1. Definitions . . . . .	4
2.2.2. Types of Differential Equations . . . . .	4
2.2.3. Extensions . . . . .	4
<b>3. Reductions &amp; Minimization</b>	<b>5</b>
<b>4. Evaluation</b>	<b>6</b>
4.1. Benchmarks . . . . .	6
<b>A. Software Requirement Specification &amp; Design Documentation</b>	<b>10</b>
A.1. Introduction . . . . .	10
A.1.1. Purpose . . . . .	10
A.1.2. Scope . . . . .	10
A.1.3. Definitions, Acronyms, Abbreviations . . . . .	10
A.1.4. Overview . . . . .	10
A.2. Overall description . . . . .	11
A.2.1. Product Perspective . . . . .	11
A.2.2. Product Functions . . . . .	11
A.2.3. User Characteristics . . . . .	11
A.2.4. Constraints . . . . .	11
A.2.5. Assumptions and Dependencies . . . . .	11
A.3. Requirement Specification . . . . .	12
A.3.1. Software System requirements . . . . .	12
A.3.2. External Requirements . . . . .	12
A.3.3. Functional requirements . . . . .	12
A.4. Proposed Software Architecture . . . . .	14
A.4.1. Overview . . . . .	14
A.4.2. Subsystem decomposition . . . . .	14
A.4.3. Interfaces . . . . .	15
A.4.4. Boundary conditions . . . . .	15

# **1. Introduction**

## **2. Models**

### **2.1. Automata**

### **2.2. Differential Equations**

#### **2.2.1. Definitions**

#### **2.2.2. Types of Differential Equations**

#### **2.2.3. Extensions**

### **3. Reductions & Minimization**

## **4. Evaluation**

### **4.1. Benchmarks**

# Bibliography

- [1] Steven Abney, David McAllester, and Fernando Pereira. "Relating probabilistic grammars and automata". In: *Proceedings of the 37th Annual Meeting of the Association for Computational Linguistics*. 1999, pp. 542–549.
- [2] Giovanni Bacci et al. "On the metric-based approximate minimization of Markov Chains". In: *Journal of Logical and Algebraic Methods in Programming* 100 (2018), pp. 36–56.
- [3] Andrea Bobbio and Kishor S. Trivedi. "An aggregation technique for the transient analysis of stiff Markov chains". In: *IEEE Transactions on computers* 9 (1986), pp. 803–814.
- [4] François Boulier et al. "Towards an automated reduction method for polynomial ODE models of biochemical reaction systems". In: *Mathematics in Computer Science* 2.3 (2009), pp. 443–464.
- [5] George Edward Briggs and John Burdon Sanderson Haldane. "A note on the kinetics of enzyme action". In: *Biochemical journal* 19.2 (1925), p. 338.
- [6] Janusz A Brzozowski. "Canonical regular expressions and minimal state graphs for definite events". In: *Mathematical theory of Automata* 12.6 (1962), pp. 529–561.
- [7] Peter Buchholz. "Bisimulation relations for weighted automata". In: *Theoretical Computer Science* 393.1-3 (2008), pp. 109–123.
- [8] Peter Buchholz. "EXACT AND ORDINARY LUMPABILITY IN FINITE MARKOV CHAINS". In: 1994.
- [9] RG Bukharaev. "Probabilistic automata". In: *Journal of Soviet Mathematics* 13.3 (1980), pp. 359–386.
- [10] Luca Cardelli et al. "Maximal aggregation of polynomial dynamical systems". In: *Proceedings of the National Academy of Sciences of the United States of America* 114 38 (2017), pp. 10029–10034.
- [11] Charles Francis Curtiss and Joseph O Hirschfelder. "Integration of stiff equations". In: *Proceedings of the National Academy of Sciences of the United States of America* 38.3 (1952), p. 235.
- [12] Pedro R DArgenio and Joost-Pieter Katoen. "A theory of stochastic systems part I: Stochastic automata". In: *Information and computation* 203.1 (2005), pp. 1–38.
- [13] Pedro R DArgenio and Joost-Pieter Katoen. "A theory of stochastic systems. Part II: Process algebra". In: *Information and Computation* 203.1 (2005), pp. 39–74.
- [14] Peter Deuflhard and Jörg Heroth. "Dynamic dimension reduction in ODE models". In: *Scientific computing in chemical engineering*. Springer, 1996, pp. 29–43.
- [15] Manfred Droste, Werner Kuich, and Heiko Vogler. *Handbook of weighted automata*. Springer Science & Business Media, 2009.
- [16] Manfred Droste and Dietrich Kuske. "Weighted automata". In: *Handbook AutoMathA* (2013).
- [17] Albert Einstein. "On the theory of the Brownian movement". In: *Ann. Phys* 19.4 (1906), pp. 371–381.
- [18] Kousha Etesami. "Analysis of probabilistic processes and automata theory". In: *Automata: from Mathematics to Applications* (2016).

- [19] Bernhard C Geiger et al. "Optimal kullback–leibler aggregation via information bottleneck". In: *IEEE Transactions on Automatic Control* 60.4 (2014), pp. 1010–1022.
- [20] Stuart Geman and Mark Johnson. "Probabilistic grammars and their applications". In: *International Encyclopedia of the Social & Behavioral Sciences* 2002 (2002), pp. 12075–12082.
- [21] G Grinstein, C Jayaprakash, and Yu He. "Statistical mechanics of probabilistic cellular automata". In: *Physical review letters* 55.23 (1985), p. 2527.
- [22] Jack K Hale et al. *Introduction to functional differential equations*. Vol. 99. Springer Science & Business Media, 1993.
- [23] Thomas Henzinger, Barbara Jobstmann, and Verena Wolf. "Formalisms for Specifying Markovian Population Models". In: vol. 22. Sept. 2009. DOI: 10.1007/978-3-642-04420-5\_2.
- [24] John Hopcroft. "An  $n \log n$  algorithm for minimizing states in a finite automaton". In: *Theory of machines and computations*. Elsevier, 1971, pp. 189–196.
- [25] Tao Jiang and Bala Ravikumar. "Minimal NFA problems are hard". In: *SIAM Journal on Computing* 22.6 (1993), pp. 1117–1141.
- [26] Tsunehiko Kameda and Peter Weiner. "On the state minimization of nondeterministic finite automata". In: *IEEE Transactions on Computers* 100.7 (1970), pp. 617–627.
- [27] Michael N Katehakis and Laurens C Smit. "A successive lumping procedure for a class of Markov chains". In: *Probability in the Engineering and Informational Sciences* 26.4 (2012), pp. 483–508.
- [28] Stefan Kiefer and Björn Wachter. "Stability and complexity of minimising probabilistic automata". In: *International Colloquium on Automata, Languages, and Programming*. Springer. 2014, pp. 268–279.
- [29] Stefan Kiefer et al. "On the Complexity of Equivalence and Minimisation for Q-weighted Automata". In: *Logical Methods in Computer Science* 9 (2013).
- [30] Peter Kunkel and Volker Mehrmann. *Differential-algebraic equations: analysis and numerical solution*. Vol. 2. European Mathematical Society, 2006.
- [31] Wilhelm Kutta. "Beitrag zur naherungsweisen integration totaler differentialgleichungen". In: *Z. Math. Phys.* 46 (1901), pp. 435–453.
- [32] Pierre-Simon Laplace. *Philosophical Essay on Probabilities: Translated from the fifth French edition of 1825*. Vol. 13. Springer Science & Business Media, 1998.
- [33] Cristopher Moore and James P Crutchfield. "Quantum automata and quantum grammars". In: *Theoretical Computer Science* 237.1-2 (2000), pp. 275–306.
- [34] Isaac Newton. "Methodus fluxionum et serierum infinitarum". In: *Opuscula mathematica, philosophica et philologica* 1 (1774), p. 1774.
- [35] Bernt Øksendal. "Stochastic differential equations". In: *Stochastic differential equations*. Springer, 2003, pp. 65–84.
- [36] Stephan Olariu and Albert Y Zomaya. "Cellular Automata, PDEs, and Pattern Formation". In: *Handbook of Bioinspired Algorithms and Applications*. Chapman and Hall/CRC, 2005, pp. 291–302.
- [37] Alan V Oppenheim. *Discrete-time signal processing*. Pearson Education India, 1999.
- [38] Steven A Orszag. "Numerical methods for the simulation of turbulence". In: *The Physics of Fluids* 12.12 (1969), pp. II–250.
- [39] Azaria Paz. *Introduction to probabilistic automata*. Academic Press, 2014.
- [40] Tatjana Petrov. "Markov chain aggregation and its application to rule-based modelling". In: *CoRR* abs/1812.09774 (2018). arXiv: 1812.09774. URL: <http://arxiv.org/abs/1812.09774>.



- [41] Linda Petzold. "Differential/Algebraic Equations Are Not ODEs". In: *SIAM J. Sci. Stat. Comput.* 3.3 (Sept. 1982), pp. 367–384. ISSN: 0196-5204. DOI: 10.1137/0903023. URL: <https://doi.org/10.1137/0903023>.
- [42] Michael O Rabin. "Probabilistic automata". In: *Information and control* 6.3 (1963), pp. 230–245.
- [43] John Rhodes, Chrystopher L Nehaniv, and Morris W Hirsch. *Applications of automata theory and algebra: via the mathematical theory of complexity to biology, physics, psychology, philosophy, and games*. World Scientific, 2010.
- [44] Jean-Pierre Richard. "Time-delay systems: an overview of some recent advances and open problems". In: *Automatica* 39.10 (2003), pp. 1667–1694. ISSN: 0005-1098. DOI: [https://doi.org/10.1016/S0005-1098\(03\)00167-5](https://doi.org/10.1016/S0005-1098(03)00167-5). URL: <http://www.sciencedirect.com/science/article/pii/S0005109803001675>.
- [45] Claus Scheiderer. *Script: Linear Algebra I*. Department of Mathematics and Statistics, University of Konstanz, 2017.
- [46] Uwe Schöning. *Theoretische Informatik-kurz gefasst*. BI-Wiss.-Verlag, 1992.
- [47] Marcel Paul Schützenberger. "On the definition of a family of automata". In: *Information and control* 4.2-3 (1961), pp. 245–270.
- [48] C. E. Shannon and J. McCarthy. *Automata Studies.(AM-34)*. Vol. 34. Princeton University Press, 1956.
- [49] George F Simmons. *Differential equations with applications and historical notes*. CRC Press, 2016.
- [50] Ana Sokolova and Erik P De Vink. "Probabilistic automata: system types, parallel composition and comparison". In: *Validation of Stochastic Systems*. Springer, 2004, pp. 1–43.
- [51] Ana Sokolova and Erik P De Vink. "Probabilistic automata: system types, parallel composition and comparison". In: *Validation of Stochastic Systems*. Springer, 2004, pp. 1–43.
- [52] Mariëlle Stoelinga. "An introduction to probabilistic automata". In: *Bulletin of the EATCS* 78.176-198 (2002), p. 2.
- [53] Stephen Strogatz. "Nonlinear dynamics and chaos: with applications to physics, biology, chemistry, and engineering (studies in nonlinearity)". In: (2001).
- [54] Robert Tarjan. "Dept-first search and linear graph algorithms". In: *Siam Journal on Computing - SIAMCOMP* 1 (Jan. 1997).
- [55] Antti Valmari and Giuliana Franceschinis. "Simple O (m logn) time Markov chain lumping". In: *International Conference on Tools and Algorithms for the Construction and Analysis of Systems*. Springer. 2010, pp. 38–52.
- [56] Nicolaas Godfried Van Kampen. *Stochastic processes in physics and chemistry*. Vol. 1. Elsevier, 1992.
- [57] Vito Volterra. "Theory of functionals and of integral and integro-differential equations". In: (1959).
- [58] John Von Neumann. *Mathematical foundations of quantum mechanics: New edition*. Princeton university press, 2018.
- [59] John Von Neumann, Arthur W Burks, et al. "Theory of self-reproducing automata". In: *IEEE Transactions on Neural Networks* 5.1 (1966), pp. 3–14.
- [60] Thorsten Wissmann et al. "From Generic Partition Refinement to Weighted Tree Automata Minimization". In: *arXiv preprint arXiv:2004.01250* (2020).
- [61] Daniel Zwillinger. *Handbook of differential equations*. Vol. 1. Gulf Professional Publishing, 1998.

# A. Software Requirement Specification & Design Documentation

## A.1. Introduction

### A.1.1. Purpose

The purpose of this Software Requirements Specification is to describe the features, constraints and demands of a tool for model reduction and minimization of stochastic dynamical systems in detail. This document is intended for both the supervisors and the developers of the tool.

### A.1.2. Scope

This software system shall implement a tool for model reduction and minimization of stochastic dynamical systems, that provides support for differential equations and automata, equivalent benchmark examples for each, at least one algorithm for the reduction of each — namely [29] and [10]. An optional feature is the implementation of a conversion algorithm between automata and differential equations, when theoretically possible.

### A.1.3. Definitions, Acronyms, Abbreviations

**Differential equation** (DE) An equation relating a function to its derivative with respect to one or more independent variable.

**Weighted automata** (WA) An automaton consisting of states and a transition function which associates a weight to each transition

**Possible DE extensions** Extensions of the differential equation framework. For details on the specifics, see section 2.2.3

**Isomorphism** A structure-preserving, revertable, i.e. bijective morphism or mapping from a domain to a codomain

### A.1.4. Overview

In the second chapter several conditions, assumptions and circumstances will be mentioned, that help characterizing the software's special use case. In the third chapter the concrete requirements are listed.

## **A.2. Overall description**

### **A.2.1. Product Perspective**

The software system shall be the practical and evaluative basis for the underlying theory, described in the previous report. Especially it shall provide an empirical basis for the analysis of equivalence of reduction techniques for DEs and the minimization of WAs, i.e. if reducing a DE using an algorithm, does one arrive at the same complexity as when minimising a weighted automaton representing the same system as the DE. For that it shall offer scalable benchmark examples, that is an example DE with an equivalent WA. Further it shall provide a base for implementing further algorithms or new methods to be developed (e.g. if an isomorphism is found between DEs and WAs a conversion tool).

### **A.2.2. Product Functions**

The system shall take a DE or a WA as input and apply one selected algorithm onto those and then output the minimized model. Further it shall be able to compare the results of a minimisation in terms of model complexity and equivalence, i.e. answer the question whether DE reduction and WA minimisation yield different representations of the same model or if one model is more complex.

### **A.2.3. User Characteristics**

For now the only user is going to be the developer in the course of the master project and thesis. When successful enough this may or may not change. This implies that maintainability and extensibility is important, if it's ever handed-over to another developer or even extended to be usable by non-developers.

### **A.2.4. Constraints**

- Run time is crucial for these algorithms to be feasible. The system shall not impose significant overhead and the implementations shall be as fast as possible
- Memory safety is important as inputs may induce infinite memory requirements that must not execute if so (else the system will crash)
- Correctness is the most important aspect of the implementation as the results will be unusable if minor errors are introduced that corrupt the reduction or minimization processes as well as comparisons and benchmarks

### **A.2.5. Assumptions and Dependencies**

to be set when dependencies are fixed

## **A.3. Requirement Specification**

### **A.3.1. Software System requirements**

The system shall be implemented with focus on the following traits:

- S 1. Correctness
- S 2. Extensibility
- S 3. Maintainability
- S 4. Lightweightness
- S 5. As fast as possible
- S 6. Memory safe for all inputs
- S 7. Cross-compileable.

### **A.3.2. External Requirements**

The system shall:

- E 1. to be set when dependencies are fixed

### **A.3.3. Functional requirements**

- F 1. Control flow system

The system shall

- 1. provide a mechanism for applying the methods depending on the specified model, i.e. apply WA validation checks, algorithm and evaluation for WA input and the respective equivalent for DEs.
- 2. provide a file based input and output mechanism.
- 3. provide a user interface based input and output mechanism.
- 4. validate the inputs before algorithm execution

- F 2. User interface

The system shall

- 1. offer 3 different methods to be applied: WA minimization, DE reduction and Benchmarking.
- 2. provide a way to specify which input method is to be used, either file-based or user interface-based.
- 3. provide a way to specify which output method is to be used.
- 4. provide the possibility to select an algorithm from a set of available ones for both models.
- 5. display the input, the output and summaries and statistics provided by the model specific modules

- F 3. WA minimization

The system shall

- 1. specify an input format for WA.
- 2. provide a validation mechanism to ensure the well-formedness of the input.
- 3. implement the algorithm specified in [29].
- 4. summarize the results and statistics on the difference between input and output.

- F 4. DE reduction

The system shall

- 1. specify an input format for arbitrary DEs and possible extensions, specifically stochastic

differential, functional differential, integro-differential and differential-algebraic equations.

2. provide a validation mechanism to ensure the well-formedness of the expression.
3. implement the algorithm specified in [10]
4. summarize the results and statistics on the difference between inputs and outputs

F 5. Benchmark The system shall

1. provide example WA and DEs, which are
  1. theoretically proven to be equivalent, see section 4.1
  2. scalable by a parameter, defining the number of states or the number of variables
2. implement a method to compare the results in terms of
  1. run time,
  2. memory
  3. resulting model complexity

F 6. Conversion or Equivalence The system shall

1. be able to convert the benchmark examples from one model to the other or to prove that instances of distinct models are equivalent
2. (Optional) be able to convert all instances of one model to the other model

## A.4. Proposed Software Architecture

### A.4.1. Overview

**Main Module** Entry point of the process, handles for the control flow.

**User Interface** Lets the user control the main module.

**Model Interface** Defines a model including format.

**Reduction Method Interface** Defines a reduction method for a specific model.

**Conversion/Equivalence Interface** Defines the conversion or equivalence notion from a specific model to a specific model.

**Benchmark Module** Defines benchmark examples and generation processes for those.

### A.4.2. Subsystem decomposition

**Main Module** The main module is the main entry point of the process, responsible for executing the user interface, the algorithms and utilities from the model specific modules, the conversions, as well as dealing with benchmark flows and loading the necessary examples. There are two mandatory basic control flows and one optional one that depends on the theoretical feasibility that is to be proven:

1. Standard model reduction for a single model with user specified input
2. Benchmark flow using the provided examples, resulting in two sequential model reduction executions. They can not be parallelized, as they would interfere with the caches and slow each other down. After the execution it converts one instance to the other model preserving model complexity or checks if they are equivalent.

**User Interface** The User Interface lets the user control the main module, provides means of input to the main module and displays the output from the main module. Also contains usage information.

A text-based user interface is to be implemented (also called command-line interface). The user interface must contain a menu letting the user specify what control flow is to be executed, thus what task the user wants to perform. It must be able to either read the data from file or from the standard input of the terminal and display the input, output and summary on the standard output of the terminal, as well as possible errors.

**Model Interface** The model interface specifies the details of a model including the format, input validation functionality, concrete instances will hold an array of function pointers of the reduction method interface type for the concrete model. Depending on the task that the user wants to perform either one or another instance is used to execute the control flow. The data flow from the user via the main module is passed to the model interface instance which does the actual processing using the defined functions and one of the functions from the array holding the model reduction method pointers. Instances of this interface must also specify how to summarize and compute statistics over the result, i.e. the differences in the model and in model complexity. To be implemented are instances for DEs and WAs.

**Reduction Method Interface** This interface is used to implement concrete reduction methods for a specific model. For each model there may be multiple reduction methods. To be implemented are the reduction methods specified in [10, 29].

**Conversion/Equivalence Interface** Using the model interfaces, implementations of this interface shall provide a method to convert an instance of a model to another model or to prove the

equivalence of two instances of different models. As of now this is a question to be further investigated in terms of theory. One open question is if there exists an isomorphism between the to be implemented methods and if so how to do the conversion or equivalence check without also transforming the model complexity (e.g. from DEs to WAs, how not to produce more or less states than there are implicitly in the DE representation). Two options are viable for implementation structurally:

1. Attach the conversions to the model interface as function pointer holding one function for each convertible model
2. Use a struct holding function pointers for equivalence/conversion in both directions

### A.4.3. Interfaces

The *AccessWebService* interface provides three functions: *getAccessToken*, *accessValid* and *access*. *getAccessToken* is used to obtain access tokens. *accessValid* checks, if the provided access token is valid. This function is used by the MSS to authenticate users. The function *access* is used to execute operations on the database. In before a authentication check is made and it is tested if the user is allowed to execute the given operation.

```
Interface AccessWebService {
public string accesstoken getAccessToken(string username, string password) {
    require username.length > 0 && password.length > 0;
    ensure database.getUser(username).accesstoken == accesstoken &&
    database.getUser(username).expirationDate;
    ensure containsLogEntry(user, system.getCurrentDate());
}

public boolean valid accessValid(string username, string accesstoken) {
    require database.existsEntry(username);
    ensure valid == database.getUser(username).isIsValidToken(accesstoken);
}

public Response r access(string username,
                        string accesstoken, Operation op) {
    require database.entryExists(username);
    ensure iff accessValid(username, accesstoken) then
    iff database.getUser(username).isLocked() then
        operation == new PasswordChangeRequiredResponse();
    else
        iff database.getUser().getPrivilegeLvl() > getPrivilegeLvl(operation) then
            operation is executed and r is the response of the operation;
        else
            r == new AccessDeniedResponse();
    ensure if accesstoken is not valid operation is not executed and r is null;
}
}
```

### A.4.4. Data and Control Flow

### A.4.5. Boundary conditions