PhD Thesis

The Pure Functional Programming Paradigm In Agent-Based Simulation

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Abstract

This thesis systematically investigates the use of the *pure* functional programming paradigm for implementing Agent-Based Simulations (ABS) and provides in-depth discussions on the benefits and drawbacks when doing so. As language of choice, Haskell is used due to its modern, *pure* nature and increasing use in real-world applications.

TODO "first draft" milestone until return to UK mid June 2019

1. LEAVE THE THESIS ASIDE FOR 2 WEEKS. then read whole thesis front to back and point out weaknesses in each chapter
2. MANDATORY, HIGH EFFORT: write "The structure of ABS computation" section: extract the foundational properties: introduce continuations and closures and show how they are used in SF and MSF to be simple immutable objects, further discuss agents as monad / comonad / arrow and discuss their implications from an abstract point of view. This requires a lot of reading and some writing.

TODO "finalise research" milestone until end of July 2019

1. MANDATORY, HIGH EFFORT: refine/rewrite event-driven implementation, it is too ad-hoc and the weakest (finished) chapter atm, see the chapter notes for more details on the rewrite. Need to give careful thought about the new structure, how we combine Sugarscape and event-driven SIR in it.
2. OPTIONAL, HIGH EFFORT: implement total SD and ABS SIR implementation in Idris on a very simple level to make the point that we can (or cannot) make use of dependent types in this context to show the totality of a simulation under given equilibrium assumption.

TODO "finalising, reflecting and filling in holes" milestone until end of August 2019

1. finalising all chapters
2. Reading: Ionescu thesis
3. Understand Ionescu: check what ionescou wants from his students and what literaure he cites, watch YouTube video
4. Refine Presentation: Has to come across as a thesis, not a technical report! Need to discuss concepts more generally and derive more concepts from the explanations, otherwise it looks like an advanced technical report.

TODO "cleaning up / polishing" milestone until end of September 2019

1. consistency of words / expressions

- avoid WE because I have written this thesis, so remove all personal references e.g. not We or I
- s vs 's vs. s' e.g. Agents vs. Agents's vs. Agents'
- case study vs. case-study (no -)
- Monad vs monad - write them UPPER case
- speedup vs speed up vs speed-up
- types / function names / monad names ITALIC!?
- main-thread vs main thread
- avoid don't, won't, haven't, e.g.,... and write them all out
- be consistent about italics: use it for types, functions and emphasising certain word

2. when citing multiple references, make sure they are in ascending order of their reference number
3. Fix all ? ref: papers and chapters
4. proof reading
5. put full implementations of existing models from phd repo in separate gitrepso. e.g. sugarscape, SIR event and time as and reconcile all code into thesis code folder?
6. extract all references of the thesis in separate file and manually fine-tune them so that they are perfect: including DOI, include link to webpage in case of a blog,...
7. put my simulations of my phd into separate git repos each

TODO prepare for viva:

1. read transformers chapters
2. read exception chapter
3. read basic libraries chapter
4. completely understand monad-transformers: what is executed in which order? what about commutativity? e.g. STM is innermost monad, will be evaluated last to get an IO but this in fact leads then to the evaluation of all the monads before because STM is able to re-run
5. come up with technical and knowledge-based questions the examiners can ask: explain Monads; explain Monad Transformers; why don't Monads compose? What are shared-nothing semantics (in messaging)?
6. come up with tricky questions about my methodology, narrative and methods, pointing out weaknesses of my approach and of my thesis:

Contents

To my parents for their unconditional love and support throughout all my life.

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Part I:

Preliminaries

Chapter 1

Introduction

The traditional approach to Agent-Based Simulation (ABS) has so far always been object-oriented, due to the influence of the seminal Sugarscape model [49], in which the authors claim "[..] object-oriented programming to be a particularly natural development environment for Sugarscape specifically and artificial societies generally [..]" (p. 179). This work established the metaphor in the ABS community, that *agents map naturally to objects* [113], which still holds up today.

This thesis challenges this metaphor and explores ways of approaching ABS through the *pure* functional programming paradigm using the language Haskell. To the best of the authors knowledge, it is the first one to do so on a *systematical* level, developing a foundation by presenting fundamental concepts and advanced features to show how to leverage the paradigms benefits [78] to make them available when implementing ABS functionally. By doing this, the thesis shows *how* to implement ABS purely functional and *why* it is of benefit of doing so, what the drawbacks are and also when a pure functional approach should *not* be used. This forms the thesis' general research question *how to implement ABS purely functional and what the benefits and drawbacks are of doing so.*

Further, this thesis claims that the ABS community needs functional programming because of its *scientific computing* nature, where results need to be reproducible and correct while simulations should be able to massively scale-up as well. Due to the primarily computational character of most ABS models, not requiring non-deterministic, asynchronous input/output (IO) or direct user-interaction, a pure functional approach should be able to directly deliver these non-functional requirements. The established object-oriented approach needs considerably high effort and might even fail to deliver these objectives due to its conceptually different approach to computing as they lack strong static typing, use mutable shared state and have implicit side-effects.

Further, we regard the functional approach as a way to think and explore ABS in a deeper way - especially to develop a deeper and more complete understanding on the computational structure underlying ABS. It is well known, that functional programming helps in structuring computation in a very clear and

precise way, leading to a deeper understanding about problems. So we also see it as a tool for developing abstractions which give us a a deeper understanding of the computational structures involved in ABS. By implementing use-cases, reflecting on them and generalising, we extract implicit knowledge and make it explicit. We hope that this undertaking is to the whole benefit of the ABS discipline and will also feed back into the traditional object-oriented implementation techniques.

Struggles with established ABS approaches are described in [10], where Axelrod reports the vulnerability of ABS to misunderstanding. Due to informal specifications of models and change requests among members of a research team bugs are very likely to be introduced. He also reported how difficult it was to reproduce the work of [8], which took the team four months due to inconsistencies between the original code and the published paper. The consequence is that counter-intuitive simulation results can lead to weeks of checking whether the code matches the model and is bug-free as reported in [9].

The same problem was reported in [86], which tried to reproduce the work of Gintis [62]. In his work, Gintis claimed to have found a mechanism in bilateral decentralized exchange, which resulted in Walrasian General Equilibrium without the neo-classical approach of a tatonement process through a central auctioneer. This was a major break-through for economics as the theory of Walrasian General Equilibrium is non-constructive as it only postulates the properties of the equilibrium [35] but does not explain the process and dynamics through which this equilibrium can be reached or constructed - Gintis seemed to have found just this process.

The authors [86] failed to reproduce the results and were only able to solve the problem by directly contacting Gintis which provided the code, the definitive formal reference [1]. It was found that there was a bug in the code leading to the unexpected results, which were seriously damaged through this error. They also reported ambiguity between the informal model description in Gintis paper and the actual implementation. This lead to a research in a functional framework for agent-based models of exchange as described in [23] which tried to give a very formal functional specification of the model which comes very close to an implementation in Haskell. The failure of Gintis was investigated more in-depth in the thesis by [51] who got access to Gintis code of [62]. They found that the code didn't follow good object-oriented design principles (all was public, code duplication) and - in accordance with [86] - discovered a number of bugs serious enough to invalidate the results.

As ABS is almost always used for scientific research, producing often breakthrough scientific results as pointed out in [10], these ABS need to be *free of bugs*, *verified against their specification*, *validated against hypotheses* and ultimately be *reproducible*. Further, Axelrod explicitly mentions that the ABS community should converge both on standards for testing the robustness of ABS and on its tools.

[1] It seems that by now, Gintis has made his code, written in Object Pascal, publicly available through his homepage `https://people.umass.edu/gintis/`

This thesis hypothesises that by using pure functional programming for implementing ABS makes the resulting simulations easier to test and verify, applicable to property-based testing, easy to add parallelism and concurrency, guaranteed to be reproducible already at compile-time, have fewer potential sources of bugs and thus can raise the level of confidence in the correctness of an implementation to a new level.

Note that this thesis is *not* about comparing the object-oriented and pure functional programming paradigm in the context of implementing ABS. Such an approach would not be fruitful, as too much ink has been spilt already over which paradigm is better / worse. There seems to be no scientific evidence supporting that either one is truly superior over the other; each has its benefits and weaknesses and this thesis aims in finding out what they are when using pure functional programming in ABS.

1.1 Contributions

1. To the best knowledge of the author, this thesis is the first to *systematically* investigate the use of the functional programming paradigm, as in Haskell, to ABS, laying out in-depth technical foundations and identifying its benefits and drawbacks. Due to the increased interest in functional concepts added to object-oriented languages in recent years (lambdas and map,filter,reduce in Java 8, rise of functional frameworks in JavaScript, Pythons functional features,...), because of its established benefits in concurrent programming, testing and software-development in general, presenting such foundational research gives this thesis significant impact. Further, the use of functional programming, which focuses on explicit data-flow representation, is a strong match to scientific computing, which is data-centric as well.

2. To the best of the knowledge of the author, this thesis is the first to show the use of Software Transactional Memory (STM) to implement concurrent ABS and its potential benefit over lock-based approaches. STM is particularly strong in pure functional programming because it can be guaranteed at compile time that retry-semantics exclude non-repeatable persistent side-effects. By showing how to employ STM it is possible to implement a simulation which allows massively large-scale ABS but without the low level difficulties of concurrent programming, making it easier and quicker to develop working and correct concurrent ABS models. The use of STM allows to approach concurrency still as a data-flow approach, without cluttering model code with concurrency semantics. This and the fact that we can sell retain certain guarantees about reproducibility when using STM, makes it a highly attractive approach to scientific computing. Further, due to the increasing need for massively large-scale ABS in recent years [100], making this possible within a purely functional approach as well, gives this thesis substantial impact.

3. To the best of the authors knowledge, this thesis is the first to present the use of property-based testing in ABS, which allows declarative specification-testing of the implemented ABS directly in code with *automated* random test-case generation. This is an addition to the established Test Driven Development process and a complementary approach to unit testing, ultimately giving the developers an additional, powerful tool to test the implementation on a more conceptual level. This should lead to simulation software which is more likely to be correct, thus making this a significant contribution with valuable impact.

4. To the best of the authors knowledge, this thesis is the first to outline the potential use of *dependent types* to Agent-Based Simulation on a *conceptual level* to investigate its usefulness for increasing the correctness of a simulation. Dependent types can help to narrow the gap between the model specification and its implementation, reducing the potential for conceptual errors in model-to-code translation. This immediately leads to fewer number of tests required due to guarantees being expressed already at compile time. Ultimately dependent types lead to higher confidence in correctness due to formal guarantees in code, making this a unique contribution with high impact.

1.2 Publications

Throughout the course of the Ph.D. five (5) papers were written and attempted to publish, out of which three (3) were accepted and published:

1. The Art Of Iterating - Update Strategies in Agent-Based Simulation [150]; submitted and accepted at the Social Simulation Conference 2017 - This paper derives four different update-strategies and their properties possible in time-driven ABS and discusses them from a programming-paradigm agnostic point of view. It is the first paper which makes the very basics of update-semantics clear on a conceptual level and is necessary to understand the options one has when implementing time-driven ABS purely functional. Chapter 3 builds heavily on the contents of this paper. Further the introduction to ABS in Chapter 2.2 is covered to a large extent already in this paper.

2. Pure Functional Epidemics [149]; submitted and accepted at the IFL Conference 2018 - Using an agent-based SIR model, this paper establishes in technical detail *how* to implement time-driven ABS in Haskell using non-monadic FRP with Yampa and monadic FRP with Dunai. It outlines benefits and drawbacks and also touches on important points which were out of scope and lack of space in this paper but which will be addressed in the Methodology chapter of this thesis. Chapter 4 is basically an identical copy of this paper, with minor extensions and restructuring. Further the

introduction to FRP in Chapter 2.3 is covered to a large extent already in this paper.

3. A Tale Of Lock-Free Agents [151]; submitted to the TOMACS Journal in October 2018 and rejected in March 2019- This paper is the first to discuss the use of Software Transactional Memory (STM) for implementing concurrent ABS both on a conceptual and on a technical level. It presents two case-studies, with the agent-based SIR model as the first and the famous SugarScape being the second one. In both case-studies it compares performance of STM and lock-based implementations in Haskell and object-oriented implementations of established languages. Although STM is now not unique to Haskell any more, this paper shows why Haskell is particularly well suited for the use of STM and is the only language which can overcome the central problem of how to prevent persistent side-effects in retry-semantics. Chapter 8 is based on the work of this paper with minor adjustments and extensions.

4. The Agents' New Cloths? Towards Pure Functional Agent-Based Simulation (TODO cite) submitted and rejected at the Summer Simulation Conference 2019 - This paper summarizes the main benefits of using pure functional programming as in Haskell to implement ABS and discusses on a conceptual level how to implement it and also what potential drawbacks are and where the use of a functional approach is not encouraged. It is written as a conceptual / review paper, which tries to "sell" pure functional programming to the agent-based community without too much technical detail and parlance where it refers to the important technical literature from where an interested reader can start. Chapter 6 follows the ideas loosely. Further the introduction to FP in Chapter 2.3 is covered to a large extent already in this paper.

5. Show Me Your Properties! The Potential Of Property-Based Testing In Agent-Based Simulation (TODO cite); submitted and accepted at the Summer Simulation Conference 2019 - This paper introduces property-based testing on a conceptual level to agent-based simulation using the agent-based SIR model and the Sugarscape model as two case-studies. All Chapters 9, 10, 11 of Part IV and the Appendix C are substantially expanded discussions of the ideas presented in this paper.

1.3 Thesis structure

The thesis is divided into 5 parts which act as the thematic narrative throughout the text followed by an Appendix .

Part I opens the thesis by laying out the necessary prerequisites necessary to understand the ideas and motivation in the rest of the thesis.

Chapter 1 introduces the problem and presents the motivation, aim and hypotheses.

Chapter 2 presents related research and discusses the background necessary to understand the rest of the thesis. It presents a definition of ABS and gives a short introduction to functional programming with advanced topics necessary to understand the concepts in this thesis. Further it discusses the methodology.

Chapter 3 discusses an architectural categorisation on how to implement ABS from a language-agnostic point of view.

Part II presents *how* to do ABS in pure functional programming.

Chapter 4 derives a time-driven ABS implementation for an agent-based SIR model. Because it is the first chapter discussing how to implement ABS pure functionally, it goes quite into detail to lay out the basic concepts.

Chapter 5 presents an event-driven approach to ABS using an event-driven agent-based SIR model the highly complex Sugarscape model. It takes up the concepts derive in the previous Chapter 4, generalises them and pushes them forward to a more generic solution. Further it also gives a brief outline how to transform the time-driven SIR implementation into an event-driven one.

Chapter 6 takes a highly abstract look at the computational approach and structures, derived in quite an ad-hoc fashion in the previous two Chapters 4, 5. It distils the essence of the SF and MSF constructs and shows that by looking at their building blocks of *closures* and *continuations*, SF and MSF can be regarded as very simple, immutable, pure functional objects. Further it looks at how they relate to existing computational structures like Monads, Comonads and Arrows.

Part III presents parallel computation in ABS as the first of two parts of *why* pure functional ABS is of benefit.

Chapter 7 shows rather briefly how to achieve deterministic and pure parallelism in pure functional ABS.

Chapter 8 presents an in-depth discussion on how to implement concurrent ABS using Software Transactional Memory.

Part IV presents property-based testing in ABS as the second of two parts of *why* pure functional ABS is of benefit.

Chapter 9 shows how to use property-based testing to implement a full agent-specification test of the event- and time-driven SIR model in code and run it as property-tests.

Chapter 10 shows how to derive and encode invariants, the dynamics of the simulation must uphold in property-tests. Further it shows how to compare the

dynamics of two implementations of the same underlying model, namely the the time- and event-driven SIR implementations.

Chapter 11 discusses how to put model specifications into code and check them with property-tests: it shows how to compare the SD simulation to the agent-based one.

Part V is the closing part which looks at the thesis as a whole, discusses and concludes.

Chapter 12 puts all parts in perspective to each other and the initial motivation and hypothesis and discusses them under these viewpoints.

Chapter 13 concludes, briefly outlines unanswered questions and presents further research.

Appendices contains additional material which relates to the overall research of this thesis but would be out of context in the respective chapters referring to it.

Appendix A shows a pure functional implementation of a System Dynamics (SD) SIR simulation using Functional Reactive Programming (FRP). It shows that we can directly encode SD specification in pure functional FRP code with extremely high guarantees in correctness. We use this implementation in Chapter 11 where we test the agent-based SIR dynamics against the SD ones.

Appendix B discusses the deep question of whether it is possible to test or guarantee that a correct implementation of the SIR model does terminate or not. This question arises in the context of Chapter 10 and 9.

Appendix C contains a brief overview over the validation process we went through when trying to get our Sugarscape implementation from Chapter 5 in line with the results from the original specification [49]. Further we show how we can use property-based testing in an exploratory model to formulate and test hypotheses.

Chapter 2

Background

2.1 Related research and literature

The amount of research on using pure functional programming with Haskell in the field of ABS has been moderate so far. Most of the papers are related to the field of Multi Agent Systems (MAS) and look into how agents can be specified using the belief-desire-intention paradigm [40, 145, 88].

A multi-method simulation library in Haskell called *Aivika 3* is described in the technical report [140]. It supports implementing Discrete Event Simulations (DES), System Dynamics and comes with basic features for event-driven ABS which is realised using DES under the hood. Further it provides functionality for adding GPSS to models and supports parallel and distributed simulations. It runs within the IO effect type for realising parallel and distributed simulation but also discusses generalising their approach to avoid running in IO.

In his master thesis [17] the author investigates Haskells' parallel and concurrency features to implement (amongst others) *HLogo*, a Haskell clone of the NetLogo [163] simulation package, focusing on using STM for a limited form of agent-interactions. *HLogo* is basically a re-implementation of NetLogos API in Haskell where agents run within the IO context and thus can also make use of STM functionality. The benchmarks show that this approach does indeed result in a speed-up especially under larger agent-populations. The authors' thesis is one of the first on ABS using Haskell. Despite the concurrency and parallel aspect, this thesis approach is rather different: it avoids IO within the agents under all costs and explore the use of STM more on a conceptual level rather than implementing an ABS library to compare our case-studies with lock-based and imperative implementations.

There exists some research [42, 155, 138] using the functional programming language Erlang [6] to implement concurrent ABS. The language is inspired by the actor model [1] and was created in 1986 by Joe Armstrong for Eriksson for developing distributed high reliability software in telecommunications. The actor model can be seen as quite influential to the development of the concept

of agents in ABS, which borrowed it from Multi Agent Systems [166]. It emphasises message-passing concurrency with share-nothing semantics (no shared state between agents), which maps nicely to functional programming concepts. The mentioned papers investigate how the actor model can be used to close the conceptual gap between agent-specifications, which focus on message-passing and their implementation. Further they show that using this kind of concurrency allows to overcome some problems of low level concurrent programming as well. Also [17] ported NetLogos API to Erlang mapping agents to concurrently running processes, which interact with each other by message-passing. With some restrictions on the agent-interactions this model worked, which shows that using concurrent message-passing for parallel ABS is at least *conceptually* feasible. Despite the natural mapping of ABS concepts to such an actor language, it leads to simulations, which despite same initial starting conditions, might result in different dynamics each time due to concurrency.

The work [100] discusses a framework, which allows to map Agent-Based Simulations to Graphics Processing Units (GPU). Amongst others they use the SugarScape model [49] and scale it up to millions of agents on very large environment grids. They reported an impressive speed-up of a factor of 9,000. Although their work is conceptually very different this thesis draws inspiration from their work in terms of performance measurement and comparison to the Sugarscape model.

Using functional programming for DES was discussed in [88] where the authors explicitly mention the paradigm of Functional Reactive Programming (FRP) to be very suitable to DES.

A domain-specific language for developing functional reactive agent-based simulations was presented in [135, 156]. This language called FRABJOUS is human readable and easily understandable by domain-experts. It is not directly implemented in FRP/Haskell but is compiled to Haskell code which they claim is also readable. This supports that FRP is a suitable approach to implement ABS in Haskell. Unfortunately, the authors do not discuss their mapping of ABS to FRP on a technical level, which would be of most interest to functional programmers.

Object-oriented programming and simulation have a long history together as the former one emereged out of Simula 67 [39], which was created for simulation purposes. Simula 67 already supported DES and was highly influential for today's object-oriented languages. Although the language was important and influential, in our research we look into different approaches, orthogonal to the existing object-oriented concepts.

Lustre is a formally defined, declarative and synchronous dataflow programming language for programming reactive systems [68]. While it has solved some issues related to implementing ABS in Haskell, it still lacks a few important features necessary for ABS. There seems to be no way of implementing an environment in Lustre as it is done in Chapters 4 and 5. Also, the language seems not to come with stochastic functions, which are but the very building blocks of ABS. Finally, Lustre does only support static networks, which is clearly a drawback in ABS in general where agents can be created and terminated dynamically

during simulation.

In [22], the authors discuss the problem of advancing time in message-driven agent-based socio-economic models. They formulate purely functional definitions for agents and their interactions through messages. Our architecture for synchronous agent-interaction as discussed in Chapter 5.1 was not directly inspired by their work but has some similarities: the use of messages and the problem of when to advance time in models which allows unrestricted synchronised agent interactions.

The authors of [23] are using functional programming as a specification for an agent-based model of exchange markets but leave the implementation for further research where they claim that it requires dependent types. This paper is the closest usage of dependent types in agent-based simulation we could find in the existing literature and to our best knowledge there exists no work on general concepts of implementing pure functional agent-based simulations with dependent types.

In his talk [146], Tim Sweeney CTO of Epic Games discussed programming languages in the development of game engines and scripting of game logic. Although the fields of games and ABS seem to be very different, Gregory [65] defines computer-games as *"[..] soft real-time interactive agent-based computer simulations"* (p. 9) and indeed, they have striking similarities: both are simulations which perform numerical computations and update objects in a loop either concurrently or sequential. In games these objects are called *game-objects* and in ABS they are called *agents* but they are conceptually the same thing. Sweeney reports that reliability suffers from dynamic failure in languages like C++ e.g. random memory overwrites, memory leaks, accessing arrays out-of-bounds, dereferencing null pointers, integer overflow, accessing uninitialized variables. He reports that 50% of all bugs in the Game Engine Middleware Unreal can be traced back to such problems and presents dependent types as a potential rescue to those problems. The two main points Sweeney made were that dependent types could solve most of the run-time failures and that parallelism is the future for performance improvement in games. He distinguishes between pure functional algorithms which can be parallelised easily in a pure functional language and updating game-objects concurrently using Software Transactional Memory (STM).

2.2 Agent-Based Simulation

This thesis understands Agent-Based Simulation (ABS) as a methodology to model and simulate a system, where the global behaviour may be unknown but the behaviour and interactions of the parts making up the system is known. Those parts, called agents, are modelled and simulated, out of which then the aggregate global behaviour of the whole system emerges. So, the central aspect of ABS is the concept of an agent, a metaphor for a pro-active unit, situated in an environment, able to spawn new agents and interacting with other agents in some neighbourhood by exchange of messages [102, 114, 139, 166]. Summarising,

this thesis informally assumes the following about agents:

- They are uniquely addressable entities with some internal state over which they have full, exclusive control.
- They are pro-active, which means they can initiate actions on their own e.g. change their internal state, send messages, create new agents, terminate themselves.
- They are situated in an environment and can interact with it.
- They can interact with other agents situated in the same environment by means of messaging.

Epstein [48] identifies ABS to be especially applicable for analysing *"spatially distributed systems of heterogeneous autonomous actors with bounded information and computing capacity"*. They exhibit the following properties:

- Linearity & Non-Linearity - actions of agents can lead to non-linear behaviour of the system.
- Time - agents act over time, which is also the source of their pro-activity.
- State - agents encapsulate some state, which can be accessed and changed during the simulation.
- Feedback-Loop - because agents act continuously and their actions influence each other and themselves in the future of subsequent time-steps, feedback-loops are a fundamental concept, inherent to every ABS.
- Heterogeneity - agents can have properties (age, height, sex,...) where the actual values can vary arbitrarily between agents.
- Interactions - agents can be modelled after interactions with an environment and other agents.
- Spatiality & Networks - agents can be situated within arbitrary environments, like spatial environments (discrete 2D, continuous 3D,...) or complex networks.

Note that there doesn't exist a commonly agreed technical definition of ABS but the field draws inspiration from the closely related field of Multi-Agent Systems (MAS) [162, 166]. It is important to understand that MAS and ABS are two different fields where in MAS the focus is much more on technical details, implementing a system of interacting intelligent agents within a highly complex environment with the focus primarily on solving AI problems.

The field of ABS can be traced back to self-replicating von Neumann machines, cellular automata and Conway's Game of Life. The famous Schelling

segregation model [134] is regarded as a pioneering example. The most prominent topics which are explored in social simulation are social norms, institutions, reputation, elections and economics.

Axelrod [9, 11] has called social simulation the third way of doing science, which he termed the *generative* approach, which is in opposition to the classical inductive (finding patterns in empirical data) and deductive (proving theorems). Thus, the generative approach can be seen as a form of empirical research and is a natural environment for studying social and interdisciplinary phenomena as discussed more in-depth in the work of Epstein [47, 48]. He gives a fundamental introduction to agent-based social social simulation and makes the strong claim that *"If you didn't grow it, you didn't explain its emergence"* [1]. Epstein puts much emphasis on the claim that ABS is indeed a scientific instrument as hypotheses which are investigated are empirical falsifiable: the simulation exhibits the emergent pattern in which case the model is *one* way of explaining it or it simply does not show the emergent pattern, in which case the hypothesis, that the model (the micro-interactions amongst the agents) generates the emergent pattern is falsified [2] - we haven't found an explanation *yet*. So in summary, growing a phenomena is a necessary, but not sufficient condition for explanation [47].

The first large scale ABS model which rose to some prominence was the *Sugarscape* model developed by Epstein and Axtell in 1996 [49]. Their aim was to *grow* an artificial society by simulation and connect observations in their simulation to phenomenon of real-world societies. It was this simulation which strongly advertised object-oriented programming to implement ABS and due to this and also due to the general popularity of object-oriented which started to rise in the early-mid 90s, it is reasonable to say that the established, state-of-the-art approach to implement ABS falls into three categories:

1. Programming from scratch using object-oriented languages with Python, Java and C++ being the most popular ones.

2. Programming using a 3rd party ABS library using object-oriented languages where RePast and DesmoJ, both in Java, are the most popular ones.

3. Using a high-level ABS tool-kit for non-programmers, which allow customization through programming if necessary. By far the most popular one is NetLogo with an imperative programming approach followed by AnyLogic with an object-oriented Java approach.

To get a deeper idea and understanding of ABS, the next sections present two different, well-known agent-based models to give examples of two different

[1] Note the fundamental constructivist approach to social science, which implies that the emergent properties are actually computable. When making connections from the simulation to reality, constructible emergence raises the question whether our existence is computable or not. When pushing this further, we can conjecture that the future of simulation will be simulated copies of our own existence, which potentially allows to simulate *everything*. This idea is not new and an interesting treatment of it can be found in [21, 141].

[2] This is fundamentally following Poppers theory of science [127].

Figure 2.1: States and transitions in the SIR compartment model.

types: the explanatory SIR model and the exploratory Sugarscape model. Both are used throughout the thesis as use-cases for developing the pure functional ABS techniques.

2.2.1 The SIR model

The *explanatory* SIR model is a very well studied and understood compartment model from epidemiology [93], which allows to simulate the dynamics of an infectious disease like influenza, tuberculosis, chicken pox, rubella and measles spreading through a population.

In this model, people in a population of size N can be in either one of the three states *Susceptible*, *Infected* or *Recovered* at a particular time, where it is assumed that initially there is at least one infected person in the population. People interact *on average* with a given rate of β other people per time-unit and become infected with a given probability γ when interacting with an infected person. When infected, a person recovers *on average* after δ time-units and is then immune to further infections. An interaction between infected persons does not lead to re-infection, thus these interactions are ignored in this model. This definition gives rise to three compartments with the transitions seen in Figure 2.1.

This model was also formalized using System Dynamics (SD) [128]. In SD one models a system through differential equations, allowing to conveniently express continuous systems, which change over time, solving them by numerically integrating over time, which gives then rise to the dynamics. The SIR model is modelled using the following equation, with the dynamics shown in Figure 2.2 .

$$\begin{aligned} \frac{\mathrm{d}S}{\mathrm{d}t} &= -infectionRate \\ \frac{\mathrm{d}I}{\mathrm{d}t} &= infectionRate - recoveryRate \\ \frac{\mathrm{d}R}{\mathrm{d}t} &= recoveryRate \end{aligned} \tag{2.1}$$

$$\begin{aligned} infectionRate &= \frac{I\beta S\gamma}{N} \\ recoveryRate &= \frac{I}{\delta} \end{aligned} \tag{2.2}$$

The approach of mapping the SIR model to an ABS is to discretize the population and model each person in the population as an individual agent. The transitions between the states are happening due to discrete events caused both

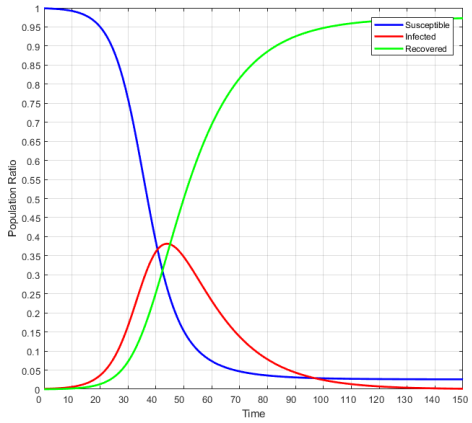


Figure 2.2: Dynamics of the SIR compartment model using the System Dynamics approach. Population Size $N = 1{,}000$, contact rate $\beta = \frac{1}{5}$, infection probability $\gamma = 0.05$, illness duration $\delta = 15$ with initially 1 infected agent. Simulation run for 150 time-steps. Generated using our pure functional SD approach (see Appendix A).

by interactions amongst the agents and timeouts. The major advantage of ABS over SD is that it allows to incorporate spatiality and simulate heterogeneity of population e.g. different sex, age. This is not directly possible with other simulation methods of SD or Discrete Event Simulation (DES) [167].

In the ABS classification of [102], this model can be seen as an *Interactive ABMS*: agents are individual heterogeneous agents with diverse set characteristics; they have autonomic, dynamic, endogenously defined behaviour; interactions happen between other agents and the environment through observed states and behaviours of other agents and the state of the environment.

2.2.2 Sugarscape

The seminal Sugarscape model was one of the first models in ABS, developed by Epstein and Axtell in 1996 [49]. Their aim was to *grow* an artificial society by simulation and connect observations in their simulation to phenomenon observed in real-world societies, making it an *exploratory* model. In the model a population of agents move around in a discrete 2D environment, where sugar and spice grows, and interact with each other and the environment in many different ways. The main features of this model are (amongst others): searching, harvesting and consuming of resources, wealth and age distributions, population dynamics under sexual reproduction, cultural processes and transmission, combat and assimilation, bilateral decentralized trading (bartering) between agents with endogenous demand and supply, disease processes transmission and immunology.

In the ABS classification of [102], the Sugarscape can be seen as an *Adaptive*

ABMS: agents are individual heterogeneous agents with diverse set characteristics; they have autonomic, dynamic, endogenously defined behaviour; interactions happen between other agents and the environment through observed states and behaviours of other agents and the state of the environment; agents can change their behaviour during the simulation through observing their own state, learning and populations can adjust their composition.

The full specification of the Sugarscape model itself fills a small book [49] of about 200 pages, so we will only give a very brief overview of the model in terms of actions which happen. Generally, the model is stepped in discrete, natural number time-steps, also called ticks, where in each tick the following actions happens:

1. Shuffle all agents and process them sequentially. The reason why the agents are shuffled is to even-out the odds of being scheduled at a specific position - it is equally probable of being scheduled in any position. The semantics of the model require to step the agents sequentially but ideally one wants to avoid any biases in ordering and pretend that agents act conceptually or statistically at the same time in parallel - the shuffling allows to do this by *running the agents sequentially which makes their behaviour appear statistically in parallel.* Every agent executes the following actions, where agents executed after the agent in the same tick, can already see the changes and interactions of preceding agents:

   (a) The agent ages by 1 tick. An agent might have a maximum age and when reached will result in the removal of the agent (see below).

   (b) Move to the nearest unoccupied site in sight with highest resource. In case of combat also sites occupied with agents from a different tribe are potential targets. Harvest all the resources on the site and in case of combat also reap the enemies resources or gather some combat reward. This is one of the primary reasons why the Sugarscape model needs to be stepped sequentially: because only one agent can occupy a site at a time, it would lead to conflicts when agents actually act at the same time.

   (c) Apply the agents' metabolism. Each agent needs to consume a given number of resources in each tick to satisfy its metabolism. The gathered resources can be stocked up during the harvesting process but if the agent does not have enough resources to satisfy its metabolism, it will be removed from the simulation (see below).

   (d) Apply pollution of the environment through the agent. Depending on how much the agent has harvested during its movement and consumed in its metabolism process, it will leave a small fraction of pollution in the environment.

   (e) Check if the agent has died from age or starved to death, in case it removes itself from the simulation and does not execute the next steps (the previous steps are executed independently from the age

of the agent). Note that depending on the model configuration this could also lead to the re-spawning of a new agent which replaces the died agent.

(f) Engage with other neighbours in mating, which involves multiple synchronous interaction-steps happening in the same tick: exchange of information and both agents agreeing on the mating action. If both agents agree to mate, the initiating agent spawns a new agent, with characteristics inherited from both parents. See Figure 2.3d.

(g) Engage in the cultural process, where cultural tags are picked up from other agents and passed on to other agents. This action is a one-way interaction where the neighbours do not reply synchronously.

(h) Engage in trading with neighbours where the initiating agent offers a given resource (sugar) in exchange for another resource (spice). The agent asks every neighbour and a trade will transact if it makes both agents better off. This action involves multiple synchronous interaction-steps within the same tick because of exchange of information and agreeing on the final transaction. See Figure 2.3d.

(i) Engage in lending and borrowing, where the agent offers loans to neighbours. This action also involves multiple synchronous interaction-steps within the same tick because of exchange of information and agreeing on the final transaction.

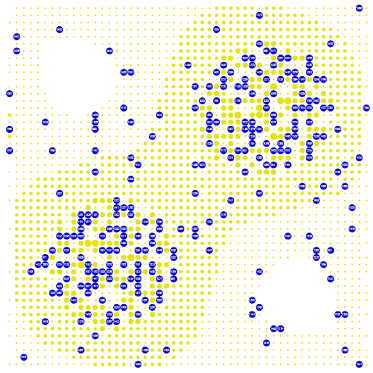
(j) Engage in disease processes, where the agent passes on diseases it has to other neighbour agents. This action is a one-way interaction where the neighbours do not reply synchronously.

2. Run the environment which consists of an NxN discrete grid

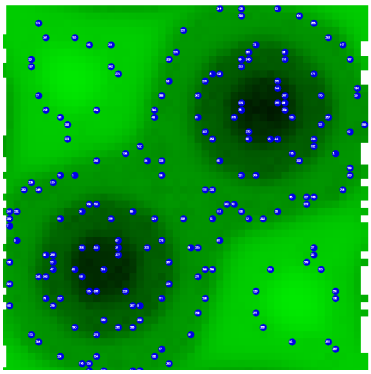
   (a) Regrow resources on each site according to the model configuration: either with a given rate per tick as seen in Figure 2.3a, or immediately. Depending on whether seasons are enabled, see Figure 2.3c, the regrowing rate varies in different regions of the environment.

   (b) Apply diffusion of pollution where the pollution generated by the agents spreads out slowly across the whole environment, see Figure 2.3b.

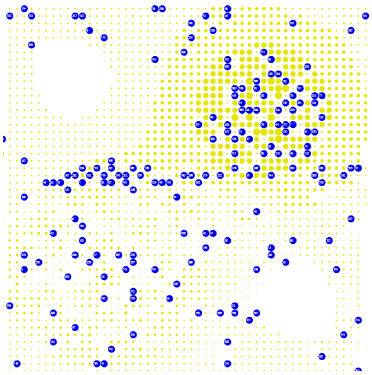
In Figure 2.3 screenshots from the Sugarscape implementation as discussed in Chapter 5.1 are shown.



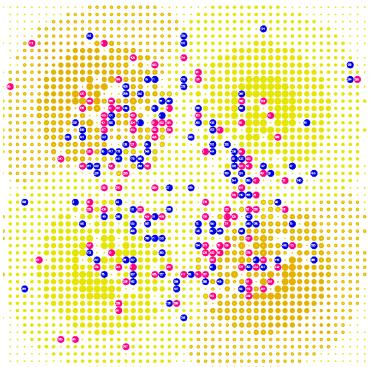
(a) *Animation II-2*: resource growback and infinite agent age.



(b) *Animation II-8*: active pollution with diffusion.



(c) *Animation II-7*: seasons, agents trying to migrate.



(d) *Figure IV-14*: trading, mating and finite life spans.

Figure 2.3: Visualisation of the Sugarscape implementation (see Chapter 5.1). The naming of the respective *Animation* and *Figure* is taken from [49].

2.3 Pure functional programming

Functional programming (FP) is called *functional* because it makes functions the main concept of programming, promoting them to first-class citizens: functions can be assigned to variables, they can be passed as arguments to other functions and they can be constructed as return values from functions. The roots of FP lie in the Lambda Calculus which was first described by Alonzo Church [30]. This is a fundamentally different approach to computing than imperative programming (including established object-orientation) which roots lie in the Turing Machine [153]. Rather than describing *how* something is computed as in the more operational approach of the Turing Machine, due to the more *declara-*

tive nature of the Lambda Calculus, code in functional programming describes *what* is computed.

In [103] the author defines FP as a methodology attributing the following properties to it: programming without the assignment-operator; allowing for higher levels of abstraction; allowing to develop executable specifications and prototype implementations; connected to computer science theory; allowing to do algebraic reasoning. Further the author makes the subtle distinction between *applicative* and *functional* programming. Applicative programming can be understood as applying values to functions where one deals with pure expressions. In those expressions the value is independent from the evaluation order, also known as referential transparency. This means that such functions have no side-effects and thus the outcome of their execution does not depend on the history or context of the system. Further, inputs and effects to an operation are obvious from the written form.

Note that applicative programming is not necessarily unique to the functional programming paradigm but can be emulated in an imperative language e.g. C as well. Functional programming is then defined by [103] as applicative programming with *higher-order* functions. These are functions which operate themselves on functions: they can take functions as arguments, construct new functions and return them as values. This is in stark contrast to the *first-order* functions as used in applicative or imperative programming which just operate on data alone. Higher-order functions allow to capture frequently recurring patterns in functional programming in the same way like imperative languages captured patterns like GOTO, while-do, if-then-else, for. Common patterns in functional programming are (amongst others) the map, fold, zip, operators. So functional programming is not really possible in this way in classic imperative languages e.g. C as you cannot construct new functions and return them as results from functions. Object-Oriented languages like Java provide mechanisms, allowing to partially work around this limitation but are still far from *pure* functional programming.

The equivalence in functional programming to the *;* operator of imperative programming, which allows to compose imperative statements, is function composition. Function composition has no side-effects as opposed to the imperative ; operator, which simply composes destructive assignment statements executed after another resulting in side-effects. At the heart of modern functional programming is monadic programming which is polymorphic function composition: one can implement a user-defined function composition by allowing to run some code in-between function composition - this code of course depends on the type of the Monad one runs in. This allows to emulate all kind of effectful programming in an imperative style within a pure functional language (see Section 2.3.2 below). Although it might seem strange following an imperative style in a pure functional language, some problems are inherently imperative in the way that computations need to be executed in a given sequence with some effects. Also a pure functional language needs to have some way to deal with effects otherwise it would never be able to interact with the outside-world and would be practically useless. The real benefit of monadic programming is that it is

explicit about side-effects and allows only effects which are fixed by the type of the monad - the side-effects which are possible are determined statically during compile-time by the type-system. Some general patterns can be extracted e.g. a map, zip, fold over monads which results in polymorphic behaviour - this is the meaning when one says that a language is polymorphic in its side-effects.

2.3.1 Language of choice

In our research we are using the *pure* FP language Haskell. The paper of [78] gives a comprehensive overview over the history of the language, how it developed and its features and is very interesting to read and get accustomed to the background of the language. The reasons for choosing Haskell are:

- Rich Feature-Set - it has all fundamental concepts of the pure FP paradigm included, of which we explain the most important ones below. Further, Haskell has influenced a large number of languages, underlining its importance and influence in programming language design.
- Real-World applications - the strength of Haskell has been proven through a vast amount of highly diverse real-world applications [79, 78], is applicable to a number of real-world problems [118] and has a large number of libraries available [3].
- Modern - Haskell is constantly evolving through its community and adapting to keep up with the fast changing field of computer science. Further, the community is the main source of high-quality libraries.
- Highly advance type system - Haskell has a strong static type system, which catches all type errors already at compile time and does not allow to bypass the type-system (unless *coerce* or other cheating functions like *unsafePerformIO* are used). Further, Haskell is a *pure* functional language and in our research it is absolutely paramount, that we focus on *pure* functional ABS, which avoids any IO type under all circumstances. This property is enabled by the advanced type system and its strong static nature.

A highly compelling example motivating the benefits of pure functional programming is the report [79], where in a prototyping contest of DARPA the Haskell prototype was by far the shortest with 85 lines of code (LoC) as compared to the C++ solution with 1105 LoC. The remarkable thing is that the Jury mistook the Haskell code as specification because its approach was to implement a small embedded domain specific language (EDSL) to solve the problem - this is a perfect proof how close an EDSL can get to a specification. When implementing an EDSL one develops and programs primitives e.g. types and functions in a host language (embed) in a way that they can be combined. The combination of these primitives then looks like a language specific to a given

[3] `https://wiki.haskell.org/Applications_and_libraries`

domain. The ease of development of EDSLs in pure functional programming is also a proof of the superior extensibility and composability of pure functional languages over object-orientation and is definitely one of its major strength. The classic paper [73] gives a wonderful way of constructing an EDSL to denotationally construct a picture reminiscent of the works of Escher. A major strength of developing an EDSL is that one can reason about and do formal verification. A nice introduction how to do reasoning in Haskell is given in [84].

It may seem that one runs into efficiency-problems in Haskell when using algorithms which are implemented in imperative languages through mutable data which allows in-place update of memory. The seminal work of [115] showed that when approaching this problem with a functional mind-set this does not necessarily be the case. The author presents functional data structures which are asymptotically as efficient as the best imperative implementations and discusses the estimation of the complexity of lazy programs.

For an excellent and widely used introduction to programming in Haskell I refer to [85]. Other, more exhaustive books on learning Haskell are [3, 99]. For an introduction to programming with the Lambda-Calculus I refer to [109]. For more general discussion of functional programming I refer to [78, 80, 103].

2.3.2 Purity and Side-Effects

Consider the factorial function in Haskell:

```
factorial :: Integer -> Integer
factorial 0 = 1
factorial n = n * factorial (n-1)
```

When looking at this function, the following can be identified:

1. Declarative - describe *what* the factorial function is rather than how to compute it. This is supported by *pattern matching* which allows to give multiple equations for the same function, matching on its input.

2. Immutable data - in FP there are no mutable variables - after a variable is assigned, it cannot change its contents. This also means that there is no destructive assignment operator which can re-assign values to a variable. To change values, recursion is employed.

3. Recursion - the function calls itself with a structurally smaller argument and will eventually reach the base case of 0. Recursion is the very meat of FP because it is the only way to implement loops in this paradigm due to immutable data.

4. Static Types - the first line indicates the name and the type of the function. In this case the function takes one Integer as input and returns an Integer as output. Types are static in Haskell which means that there can be no type errors at run-time e.g. when one tries to implicitly cast one type into another because this is not supported by this kind of type system.

5. Explicit input and output - all data which are required and produced by the function have to be explicitly passed in and out of it. There exists no global mutable data whatsoever and data-flow is always explicit.

6. Referential transparency - calling this function with the same argument will *always* lead to the same result, meaning one can replace this function by its value. This means that when implementing this function one can not read from a file or open a connection to a server. This is also known as *purity* and is indicated in Haskell in the types which means that it is also guaranteed by the compiler.

One of the fundamental strengths of Haskell is its way of dealing with side-effects in functions. A function with side-effects has observable interactions with some state outside of its explicit scope. This means that its behaviour depends on the history of the system and that it loses its referential transparency character, which makes understanding and debugging much harder. Examples for side-effects are (amongst others): modifying state, await an input from the keyboard, read or write to a file, open a connection to a server, drawing random-numbers,...

Obviously, to write real-world programs which interact with the outside world needs side-effects. Haskell allows to indicate in the *type* of a function that it does or does *not* have side-effects. Further, there are a broad range of different effect types available, to restrict the possible effects a function can have to only the required type. This is then ensured by the compiler, which means that when trying to read from a file in a function which only allows drawing random-numbers, will fail to compile. The most common side-effect types are: *IO* allows all kind of I/O related side-effects: reading/writing a file, creating threads, write to the standard output, read from the keyboard, opening network-connections, mutable references; *Rand* allows drawing random-numbers; *Reader / Writer / State* allows to read / write / both from / to an environment.

A function without any side-effect type is called *pure*, and the *factorial* function discussed above is indeed pure. Below we give an example of a function which is not pure. The *queryUser* function *constructs* a computation which, when executed, asks the user for its user-name and compares it with a given user-configuration. In case the user-name matches it returns True, and False otherwise after printing a corresponding message.

```
queryUser :: String -> IO Bool
queryUser username = do
  -- print text to console
  putStr "Type in user-name: "
  -- wait for user-input
  str <- getLine
  -- check if input matches user-name
  if str == username
    then do
      putStrLn "Welcome!"
      return True
    else do
```

```
    putStrLn "Wrong user-name!"
    return False
```

The *IO* in the first line indicates that the function runs in the IO effect and can thus (amongst others) print to the console and read input from it. What seems striking is that this looks very much like imperative code - this is no accident and intended. When we are dealing with side-effects, ordering becomes important, thus Haskell introduced the so-called *do* notation which emulates an imperative style of programming. Whereas in imperative programming languages like C, commands are chained or composed together using the ; operator, in functional programming this is done using function composition: feeding the output of a function directly into the next function. The machinery behind the *do* notation does exactly this and desugars this imperative-style code into function compositions which run custom code between each line, depending on the type of effect the computation runs in. This approach of function composition with custom code in between each function allows to emulate a broad range of imperative-style effects, including the above mentioned ones. For a technical, in-depth discussion of the concept of side-effects and how they are implemented in Haskell using Monads, I refer to the following papers: [91, 110, 157, 158, 159].

Although it might seem very restrictive at first, we get a number of benefits from making the type of effects we can use in the function explicit. First, we can restrict the side-effects a function can have to a very specific type which is guaranteed at compile time. This means we can have much stronger guarantees about our program and the absence of potential errors already at compile-time. Second, because running effects themselves is *pure*, we can execute effectful functions in a very controlled way by making the effect-context explicit in the parameters to the effect execution. This allows a much easier approach to isolated testing because the history of the system is made explicit.

A note on effect execution: it is important to understand that the code fragments of effectful computations are in fact made up of enclosing lambda expressions, with the *do* notation being a syntactic sugared version. Thus functions which have an effect in their type can be seen as *pure* functions, which are referentially transparent and return such a fragment. This fragment, also often called *action*, results in an effect and a result when executed. We have to distinguish between the execution of pure effects like Rand,Read,Write,State and the impure effect of IO. Pure effects are executed using special runner functions. They take an action together with initial values defining the history / context of the effect e.g. an initial value for the State or the read-only value of the Reader, and run the action and return their result value. Thus, these pure effects can be executed in a referential transparent and completely controlled way. The impure IO effect works different: there exists no dedicated IO execution function but it can only be executed from within the root IO action, which emanates from the *main :: IO ()* function of each Haskell program. Thus IO actions can only be run within an enclosing IO action, with the main IO action ultimately being executed by the Haskell Runtime which is linked against the executable. The reason for that is that if we would have a way of executing IO

actions within pure code we would lose all guarantees about referential transparency. There exists indeed the function *unsafePerformIO :: IO a → a*, which allows to execute an IO action within a pure function but its use is very limited and highly discouraged. Throughout this thesis and in all our code we have avoided the use of this function under all costs and it is not used anywhere.

2.3.2.1 Stacking effects using Transformers

Often it is necessary to have multiple effects available, for example we want to manipulate a global state, write to some logging mechanism and need to be able to draw random numbers. The way this is achieved in Haskell is by using Monad Transformers [90], for which Haskell provides the two libraries *mtl* and *transformers*, which basically achieve the same things with slightly different philosophies. In our approach we primarily use *mtl* as it allows to overload functions with monadic typeclasses as explained below.

Although Monads share a common interface and properties, it is not possible to compose Monads in a general way as each monad has different internals and thus it always depends on the Monad how to compose it into another arbitrary Monad [4]. Thus, the *mtl* library provides so called transformer implementations of each of the standard Monads. A transformer has an additional type parameter in its type-constructor which has to be a Monad or another Transformer. This allows to stack multiple Monads/Transformers on top of each other. The stack is closed by using a normal Monad. Note that in *mtl* all non-transformer Monads are actually transformers with the Identity Monad as type parameter e.g. *State Int* is *StateT Int Identity*. Access to the various layers of the stack is achieved with the *lift* function. Lets look at how we can define the type of a function which has multiple effects available:

```
data SimState = SimState
  { simStateAgents :: [SimAgent]
  ...
  }

simulationCore :: RandomGen g
               => Time
               -> StateT SimState (WriterT [String] (Rand g)) SimOut
simulationCore t = do
  -- get the agents from the simulation state
  -- encapsulated in StateT SimState
  as <- gets simStateAgents

  -- writing a logging output to the WriterT [String]
  -- here we need 1 lift
  lift (tell ["Next step " ++ show t])

  -- shuffle agents by running the MonadRandom action using the
  -- Rand Monad, need 2 lifts as it is the outermost monad
  asShuf <- lift $ lift $ randomShuffle as
```

[4] The technical details are quite involved but we don't go into that here and refer to the respective literature and tutorials on Monad Transformers

```
  let simOut = ...

  return simOut

randomShuffle :: MonadRandom m => [a] -> m [a]
```

The Monad stack consists of three effects: the *StateT* with *SimState* as its internal state as the innermost Monad. Note that although in the types it is the outermost, in terms of the transformer stack it is the innermost, requiring no *lift* to access. *WriterT* with *[String]* as the logging facility is a parameter to the *StateT* transformer, making it the second effect in the stack, thus requiring one *lift*. The stack is closed using the *Rand* Monad, which is the outermost effect, requiring two *lifts* to access it.

Note the use of *randomShuffle* and its type. It is an overloaded function, which has the *MonadRandom* typeclass in its type-constraints. This indicates that it is a monadic action where *m* is of type *MonadRandom*, which supports the same functionality as *Rand*. This is the major benefit *mtl* provides, which often results in much cleaner function types and does not require to fix the order of the Monads in the stacks. Another benefit is that we do not need lifts any more; the drawback is that we cannot have multiple Monads of the same type which would be still possible in a fully qualified Monad stack. The benefits becomes particularly clear when more than one effect is required, for example we could have written the type of *simulationCore*

```
simulationCore :: (MonadState SimState m, MonadWriter [String] m, MonadRandom m)
               => Time -> m SimOut
```

A final note on commutativity on Monad Transformers: because we are stacking effects on top of each other, subsequent effects can change the final outcome, depending on their position within the stack - this is called commutativity of Monads. All the Monads in the example above commute, which means it does not matter where they are positioned in the stack, the outcome will be the same. An exception to this is the *MaybeT* transformer, which introduces failure as an effect within a stack, thus when failure occurs, subsequent effects will not be applied any more, making *MaybeT* non-commutative.

2.3.3 Functional Reactive Programming

Functional Reactive Programming (FRP) is a way to implement systems with continuous and discrete time-semantics in pure functional languages. There are many different approaches and implementations but in this thesis *Arrowized* FRP [81, 82] as implemented in the library Yampa [37, 77, 111] is used.

The central concept in Arrowized FRP is the Signal Function (SF), which can be understood as a *process over time* which maps an input- to an output-signal. A signal can be understood as a value which varies over time. Thus, signal functions have an awareness of the passing of time by having access to Δt which are positive time-steps, the system is sampled with.

$$Signal\,\alpha \approx Time \to \alpha$$
$$SF\,\alpha\,\beta \approx Signal\,\alpha \to Signal\,\beta$$

Yampa provides a number of combinators for expressing time-semantics, events and state-changes of the system. They allow to change system behaviour in case of events, run signal functions and generate stochastic events and random-number streams. Below, the relevant combinators and concepts used throughout the thesis are discuss briefly. For a more in-depth discussion I refer to [37, 77, 111].

Event An event in FRP is an occurrence at a specific point in time, which has no duration e.g. the recovery of an infected agent. Yampa represents events through the *Event* type, which is programmatically equivalent to the *Maybe* type.

Dynamic behaviour To change the behaviour of a signal function at an occurrence of an event during run-time, (amongst others) the combinator *switch :: SF a (b, Event c) → (c → SF a b) → SF a b* is provided. It takes a signal function, which is run until it generates an event. When this event occurs, the function in the second argument is evaluated, which receives the data of the event and has to return the new signal function, which will then replace the previous one. Note that the semantics of *switch* are that the signal function, into which is switched, is also executed at the time of switching.

Randomness In ABS, often there is the need to generate stochastic events, which occur based on e.g. an exponential distribution. Yampa provides the combinator *occasionally :: RandomGen g ⇒ g → Time → b → SF a (Event b)* for this. It takes a random-number generator, a rate and a value the stochastic event will carry. It generates events on average with the given rate. Note that at most one event will be generated and no 'backlog' is kept. This means that when this function is not sampled with a sufficiently high frequency, depending on the rate, it will lose events.

Yampa also provides the combinator *noise :: (RandomGen g, Random b) ⇒ g → SF a b*, which generates a stream of noise by returning a random number in the default range for the type *b*.

Running signal functions To *purely* run a signal function Yampa provides the function *embed :: SF a b → (a, [(DTime, Maybe a)]) → [b]*, which allows to run an SF for a given number of steps where in each step one provides the Δt and an input *a*. The function then returns the output of the signal function for each step. Note that the input is optional, indicated by *Maybe*. In the first step at $t = 0$, the initial *a* is applied and whenever the input is *Nothing* in subsequent steps, the last *a* which was not *Nothing* is re-used.

2.3.4 Arrowized programming

Yampa's signal functions are arrows, requiring us to program with arrows. Arrows are a generalisation of monads, which in addition to the already familiar parameterisation over the output type, allow parameterisation over their input type as well [81, 82].

In general, arrows can be understood to be computations that represent processes, which have an input of a specific type, process it and output a new type. This is the reason why Yampa is using arrows to represent their signal functions: the concept of processes, which signal functions are, maps naturally to arrows.

There exists a number of arrow combinators, which allow arrowized programing in a point-free style but due to lack of space we will not discuss them here. Instead we make use of Paterson's *do* notation for arrows [119], which makes code more readable as it allows us to program with points.

To show how arrowized programming works, we implement a simple signal function, which calculates the acceleration of a falling mass on its vertical axis as an example [123].

```
fallingMass :: Double -> Double -> SF () Double
fallingMass p0 v0 = proc _ -> do
  v <- arr (+v0) <<< integral -< (-9.8)
  p <- arr (+p0) <<< integral -< v
  returnA -< p
```

To create an arrow, the *proc* keyword is used, which binds a variable after which the *do* of Patersons *do* notation [119] follows. Using the signal function *integral :: SF v v* of Yampa, which integrates the input value over time using the rectangle rule, we calculate the current velocity and the position based on the initial position *p0* and velocity *v0*. The <<< is one of the arrow combinators, which composes two arrow computations and *arr* simply lifts a pure function into an arrow. To pass an input to an arrow, $-<$ is used and $<-$ to bind the result of an arrow computation to a variable. Finally to return a value from an arrow, *returnA* is used.

2.3.5 Monadic Stream Functions

Monadic Stream Functions (MSF) are a generalisation of Yampa's signal functions with additional combinators to control and stack side effects. An MSF is a polymorphic type and an evaluation function, which applies an MSF to an input and returns an output and a continuation, both in a monadic context [121, 122]:

```
newtype MSF m a b = MSF {unMSF :: MSF m a b -> a -> m (b, MSF m a b)}
```

MSFs are also arrows, which means we can apply arrowized programming with Patersons *do* notation as well. MSFs are implemented in Dunai, which is available on Hackage. Dunai allows us to apply monadic transformations to every sample by means of combinators like *arrM :: Monad* $m \Rightarrow (a \rightarrow m\ b) \rightarrow$

MSF m a b and *arrM_ :: Monad m ⇒ m b → MSF m a b*. A part of the library Dunai is BearRiver, a wrapper, which re-implements Yampa on top of Dunai, which enables one to run arbitrary monadic computations in a signal function. BearRiver simply adds a monadic parameter m to each SF, which indicates the monadic context this signal function runs in.

To show how arrowized programming with MSFs works, we extend the falling mass example from above to incorporate monads. In this (artificial) example we assume that in each step we want to accelerate our velocity v not by the gravity constant any more but by a random number in the range of 0 to 9.81. Further we want to count the number of steps it takes us to hit the floor, that is when position p is less than 0. Also when hitting the floor we want to print a debug message to the console with the velocity by which the mass has hit the floor and how many steps it took.

We define a corresponding Monad stack with *IO* as the outermost Monad, followed by a *RandT* transformer for drawing random-numbers and finally a *StateT* transformer as innermost Monad, to count the number of steps we compute. We can access the monadic functions using *arrM* in case we need to pass an argument and *_arrM* in case no argument to the monadic function is needed:

```
type FallingMassStack g = StateT Int (RandT g IO)
type FallingMassMSF g   = SF (FallingMassStack g) () Double

fallingMassMSF :: RandomGen g => Double -> Double -> FallingMassMSF g
fallingMassMSF v0 p0 = proc _ -> do
  -- drawing random number for our gravity range
  r <- arrM_ (lift $ lift $ getRandomR (0, 9.81)) -< ()
  v <- arr (+v0) <<< integral -< (-r)
  p <- arr (+p0) <<< integral -< v
  -- count steps
  arrM_ (lift (modify (+1))) -< ()
  if p > 0
    then returnA -< p
    -- we have hit the floor
    else do
      -- get number of steps
      s <- arrM_ (lift get) -< ()
      -- write to console
      arrM (liftIO . putStrLn) -< "hit floor with v " ++ show v ++
                                  " after " ++ show s ++ " steps"
      returnA -< p
```

To run the *fallingMassMSF* function until it hits the floor we proceed as follows:

```
runMSF :: RandomGen g => g -> Int -> FallingMassMSF g -> IO ()
runMSF g s msf = do
  let msfReaderT = unMSF msf ()
      msfStateT  = runReaderT msfReaderT 0.1
      msfRand    = runStateT msfStateT s
      msfIO      = runRandT msfRand g
  (((p, msf'), s'), g') <- msfIO
  when (p > 0) (runMSF g' s' msf')
```

Dunai does not know about time in MSFs, which is exactly what BearRiver builds on top of MSFs. It does so by adding a *ReaderT Double*, which carries the Δt. This is the reason why we need one extra lift for accessing *StateT* and *RandT*. Thus *unMSF* returns a computation in the *ReaderT Double* Monad, which we need to peel away using *runReaderT*. This then results in a *StateT Int* computation, which we evaluate by using *runStateT* and the current number of steps as state. This then results in another monadic computation of *RandT* Monad, which we evaluate using *runRandT*. This finally returns an *IO* computation, which we simply evaluate to arrive at the final result.

2.4 Methodology

In this section we briefly motivate and justify our methods, to point out the scientific approach used in this thesis to address the aims and answer hypotheses put forward in Chapter 1. Fundamentally, the method we use is developing concepts step-by-step using the two well known agent-based models SIR, introduced in Chapter 2.2.1 and Sugarscape, introduced in Chapter 2.2.2. We put our approach into a broader context of how to implement ABS from a programming language agnostic view, discussed in Chapter 3, which serves as underlying assumptions and general direction to follow.

The first part of our method is dedicated to answer the question of how to implement ABS in a pure functional way, following a time-driven approach in Chapter 4 and an event-driven approach in Chapter 4. The reason for two techniques is that both are equally important in ABS and also that the concepts of event-driven ABS build on the ones developed in the preceding time-driven approach.

Generally, in both approaches, the aim is to develop a robust, maintainable and extensible implementation of the use-case models through which we develop concepts which can be adopted to ABS in general. The overall goal is a clear representation of agents with their local (immutable) state, a way for the agents to interact with an (active) environment and one-directional and synchronous interactions between agents.

The second part of our method is dedicated to show the benefits of using the previously developed pure functional approach to ABS. It is split into two parts where in the first we investigate the hypothesis that pure functional programming makes it easy to apply parallel computation using parallelism and concurrency to ABS. The second part answers another central hypothesis namely that randomize property-based testing is a good match to test stochastic ABS implementations. In both parts we apply the concepts in questions directly to the implementations developed in the previous part and look at the resulting code, performance and implications to judge whether the outcome has the expected benefit or not as stated in the hypotheses.

Generally, all concepts we derive are driven by the hypotheses and aims from the introduction and we continuously refer back to them, especially in the respective discussions and the final conclusion and discussion chapters. By

doing this we are able to qualitatively assess whether the thesis has achieved the initial aims and answered the hypotheses in a satisfactory way.

Chapter 3

Implementing ABS

In this Chapter we briefly discuss general problems and considerations, ABS implementations need to solve, independent from the programming paradigm. In general, an ABS implementation must solve the following fundamental problems:

1. How to represent an agent, its local state and its interface.
2. How to represent agent-to-agent interactions and defining and enforcing their semantics.
3. How to represent an environment.
4. How to represent agent-to-environment interactions and defining and enforcing their semantics.
5. How agents and an environment can initiate actions without external stimuli.
6. How to step the simulation.

We argue that the most fundamental concept of ABS is the *pro-activity* of both, agents and its environment. In computer systems, pro-activity, the ability to initiate actions on its own without external stimuli, is only possible when there is some internal stimulus, most naturally represented by a continuous increasing time-flow. Due to the discrete nature of computer systems, this time-flow must be discretized in steps as well and each step must be made available to the agent, acting as the internal stimulus. This allows the agent then to perceive time and become pro-active depending on time. So we can understand an ABS as a discrete time-simulation where time is broken down into continuous, real-valued or discrete natural-valued time-steps. Independent of the representation of the time-flow we have the two fundamental choices whether the time-flow is local to the agent or whether it is a system-global time-flow. Time-flows in computer-systems can only be created through threads of execution where there

are two ways of feeding time-flow into an agent. Either it has its own thread-of-execution or the system creates the illusion of its own thread-of-execution by sharing the global thread sequentially among the agents where an agent has to yield the execution back after it has executed its step. Note the similarity to an operating system with cooperative multitasking in the latter case and real multi-processing in the former.

Generally, there exist time- and event-driven approaches to ABS [108]. In time-driven ABS, time is explicitly modelled and is the main driver of the ABS dynamics. The semantics of models using this approach, center around time. As a representative example, which will be used in Chapter 4 on time-driven ABS, we use the agent-based SIR model [101, 149]. Often such models are inspired by an underlying System Dynamics approach, where the continuous time-flow is the main driving force of the dynamics. It is clear that almost every ABS models time in some way, after all, this is the very heart of Simulation: modelling a virtual system over some (virtual) time. Still we want to distinguish clearly between different semantics of time-representation in ABS: when time is seen as a continuous flow such as in the example of the agent-based SIR model, we talk about a truly time-driven approach. In other words: if an agent behaves as a time-signal then we speak of a time-driven approach. This means that if the system is sampled with a $\Delta t = 0$ then, even though the agents are executed their behaviour must stay constant and must not change.

In the case where time advances in a discrete way either by means of events or messages, we talk about an event-driven approach. As a representative example, which will be used in Chapter 5 on event-driven ABS, we use the Sugarscape model. In this model time is discrete and represented by the natural numbers where agents act in every tick - time is not modelled explicitly as in the agent-based SIR case. In such a model, the underlying semantics map more naturally to a DES core, extended by ABS features. Although the Sugarscape model does not semantically map to a DES core in a strict sense, our implementation approach is very close to such and can be easily extended to a true DES core - thus it serves as a good example for the discussion of the event-driven approach. Further, using an event-driven SIR implementation, we also show how to extend it to a pure DES core, allowing to implement models with more explicit event-driven semantics as discussed in [108].

According to the definition of ABS in Chapter 2.2, an agent is a uniquely addressable entity with an identity, an internal state it has exclusive control over and can be interacted with by means of messages. In the established object-oriented approaches to ABS all this is implemented naturally by the use of objects: an object has a clear identity, encapsulates internal state and exposes an interface through public methods through which objects can interact with each other, also called messaging. The same applies to the environment and it is by no means clear how to achieve this in a pure functional approach where we don't have objects available - this will be addressed in the subsequent Chapters 4 and 5.

Before we look into pure functional ABS implementation concepts in the next chapters, we need to discuss the concept of update strategies [150]. Generally,

there are four strategies to approach time-driven ABS, where the differences deal with how the simulation is stepped, the agents are executed and the interaction semantics work.

3.1 Sequential Strategy

In this strategy there exists a globally synchronized time-flow and in each time-step the simulation iterates through all the agents and updates one agent after another. Messages sent and changes to the environment made by agents are visible immediately, meaning that if an agent sends messages to other agents or changes the environment, agents which are executed after this agent will see these changes within the same time-step. There is no source of randomness and non-determinism, rendering this strategy to be completely deterministic in each step. Messages can be processed either immediately or queued depending on the semantics of the model. If the model requires to process the messages immediately the model must be free of potential infinite-loops. Often in such models, the agents are shuffled when the model semantics require to average out the advantage of being executed as first. This strategy is of fundamental importance for event-driven ABS in Chapter 5. See Figure 3.1 for a visualisation of the control flow in this strategy.

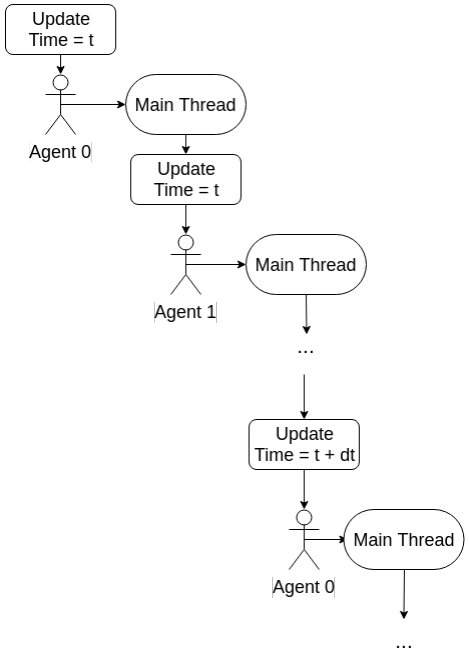


Figure 3.1: Control flow in the Sequential Strategy.

3.2 Parallel Strategy

This strategy has a globally synchronized time-flow and in each time-step iterates through all the agents and updates them in parallel. Messages sent and changes to the environment made by agents are visible in the next global step. We can think about this strategy in a way that all agents make their moves at the same time. If one wants to change the environment in a way that it would be visible to other agents this is regarded as a semantic error in this strategy. First, it is not logical because all actions are meant to happen at the same time and second, it would implicitly induce an ordering, violating the semantics of the model, the *happens at the same time* idea. It does not make a difference if the agents are really executed in parallel or just sequentially - due to the isolation of information, this has the same effect. Also it will make no difference if we iterate over the agents sequentially or randomly, the outcome has to be the same: the strategy is event-ordering invariant as all events and updates happen *virtually at the same time*. This strategy is of fundamental importance for time-driven ABS in Chapter 4. See Figure 3.2 for a visualisation of the control flow in this strategy.

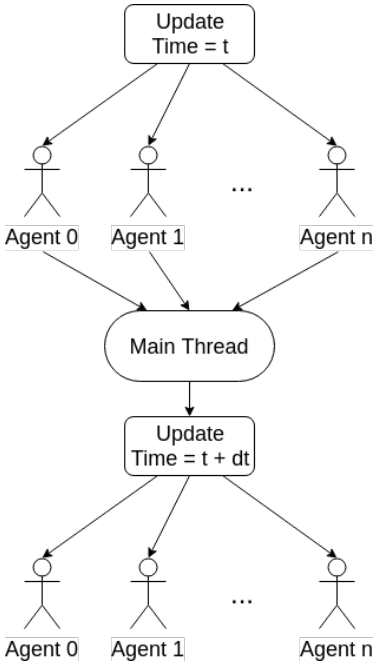


Figure 3.2: Control flow in the Parallel Strategy.

3.3 Concurrent Strategy

This strategy has a globally synchronized time-flow but in each time-step all the agents are updated in parallel with messages sent and changes to the environment are visible immediately. So this strategy can be understood as a more general form of the *parallel strategy*: all agents run at the same time but act concurrently. It is important to realize that when running agents, which are able to see actions by others immediately, in parallel, we arrive at the very definition of concurrency: parallel execution with mutual read/write access to shared data. Of course this shared data-access needs to be synchronized which in turn will introduce event-orderings in the execution of the agents. At this point we have a source of inherent non-determinism: although when one ignores any hardware-model of concurrency, at some point we need arbitration to decide which agent gets first access to a shared resource, arriving at non-deterministic solutions. This has the very important consequence that repeated runs with the same configuration of the agents and the model may lead to different results. This strategy is of fundamental importance for concurrent ABS in Chapter 8. See Figure 3.3 for a visualisation of the control flow in this strategy.

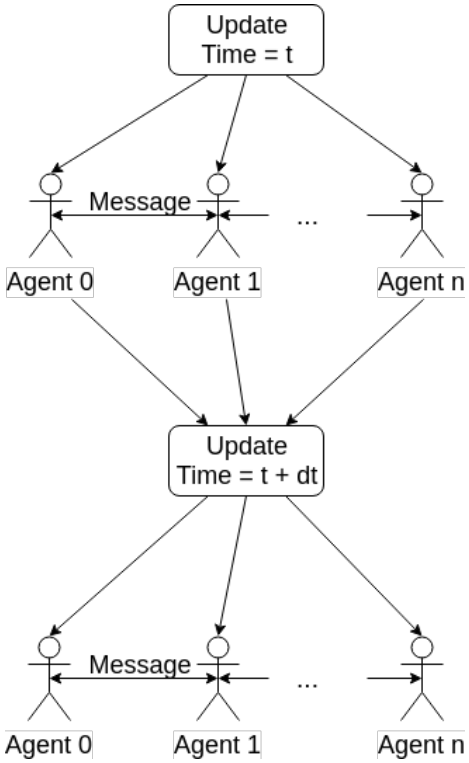


Figure 3.3: Control flow in the Concurrent Strategy.

3.4 Actor Strategy

This strategy has no globally synchronized time-flow but all the agents run concurrently in parallel, with their own local time-flow. The messages and changes to the environment are visible as soon as the data arrive at the local agents - this can be immediately when running locally on a multi-processor or with a significant delay when running in a cluster over a network. Obviously this is also a non-deterministic strategy and repeated runs with the same agent- and model-configuration may (and will) lead to different results. It is of most importance to note that information and also time in this strategy is always local to an agent as each agent progresses in its own speed through the simulation. In this case one needs to explicitly *observe* an agent when one wants to e.g. visualize it. This observation is then only valid for this current point in time, local to the observer but not to the agent itself, which may have changed immediately after the observation. This implies that we need to sample our agents with observations when wanting to visualize them, which would inherently lead to well known sampling issues. A solution would be to invert the problem and create an observer-agent which is known to all agents where each agent sends a *'I have changed'* message with the necessary information to the observer if it has changed its internal state. This also does not guarantee that the observations will really reflect the actual state the agent is in but is a remedy against the notorious sampling. The concept of Actors was proposed by [76] for which [66] and [34] developed semantics of different kinds. These works were very influential in the development of the concepts of agents and and can be regarded as foundational basics for ABS. We come back to this strategy in the context of concurrent ABS in Chapter 8. See Figure 3.4 for a visualisation of the control flow in this strategy.

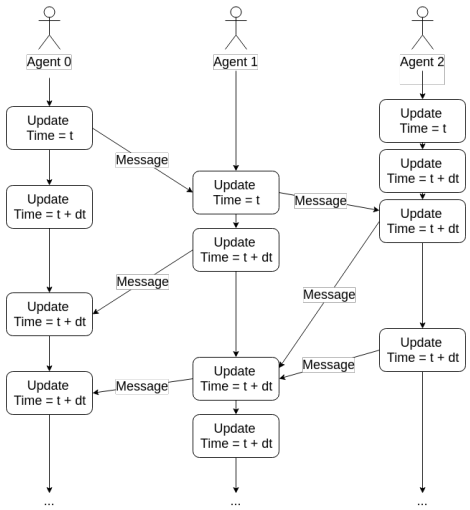


Figure 3.4: Control flow in the Actor Strategy.

3.5 Discussion

In the following chapters we discuss *how* to implement ABS from a pure functional perspective and *why* one would do so. More specifically, we show how to approach the problems discussed in this using pure functional programming (FP). The *sequential* strategy will be covered in-depth in Chapter 5 on event-driven ABS, the *parallel* one in Chapter 4 on time-driven ABS and the *concurrent* strategy is used in Chapter 8 on concurrent ABS. The *actor* strategy is not used in this thesis but its implementation follows directly from the Chapters 4 and III: instead of globally synchronising in the main-thread, a closed feedback-loop is run in every agent thread.

As already outlined in Chapter 2.2, the established approaches implementing ABS use object-oriented programming and thus solve the problems outlined at the start of this chapter from this perspective, which is quite well understood by now, as high quality ABS frameworks like RePast [112] prove. In object-oriented programming an agent is mapped directly onto an object, encapsulating the agents state and providing methods, which implement the agents' actions. Object-orientation allows to expose a well-defined interface using public methods by which one can interact with the agent and query information from it. Agent objects can directly invoke other agents' methods, implicitly mutating the other agents' internal state, which makes direct agent interaction straight forward. Also with object-orientation, agents have global access to an environment e.g. through a Singleton or a simple global variable, and can mutate the environments data by direct method calls.

All these language features are not available in FP and compare to object-orientation we face seemingly severe restrictions like immutable state, recursion and a static type system. Further, we restrict ourselves deliberately to *pure* FP and avoid running in the non-deterministic *IO* context under all costs. The question is then how to solve these problems in FP *and* use the restrictions to our advantage. In the next two chapters we show how to implement both a time-driven ABS using the agent-based SIR model as example (Chapter 4) and an event-driven ABS using the Sugarscape model as example (Chapter 5). In both we present fundamental concepts of how to engineer an ABS from a pure FP perspective. This will then be used in subsequent chapters to discuss *why* one would follow an FP approach, identifying its benefits, advantages and also drawbacks over object-oriented approaches.

Part II:

Towards pure functional ABS

Chapter 4

Pure Functional Time-Driven ABS

In this chapter, we pose solutions to the previously mentioned problems by derive a pure functional approach for time-driven ABS through the example of the agent-based SIR model. We start out with a first approach in Yampa and show its limitations. Then we generalise it to a more powerful approach, which utilises Monadic Stream Functions (MSF), a generalisation of FRP. Finally we add a structured environment, making the example more interesting and showing the real strength of ABS over other simulation methodologies like System Dynamics and Discrete Event Simulation [1].

4.1 First step: pure computation

As described in Chapter 2.3.3, Arrowized FRP [81] is a way to implement systems with continuous and discrete time-semantics where the central concept is the signal function, which can be understood as a process over time, mapping an input- to an output-signal. Technically speaking, a signal function is a continuation which allows to capture state using closures and hides away the Δt, which means that it is never exposed explicitly to the programmer, meaning it cannot be manipulated. As already pointed out, agents need to perceive time, which means that the concept of processes over time is an ideal match for our agents and our system as a whole, thus we will implement them and the whole system as signal functions.

According to the model, every agent makes *on average* contact with β random other agents per time unit. In ABS we can only contact discrete agents thus we model this by generating a random event on average every $\frac{1}{\beta}$ time units. We need to sample from an exponential distribution because the rate is propor-

[1] The code of all steps can be accessed freely through the following URL: `https://github.com/thalerjonathan/phd/tree/master/public/purefunctionalepidemics/code`

tional to the size of the population [20]. Note that an agent does not know the other agents' state when making contact with it, thus we need a mechanism in which agents reveal their state in which they are in *at the moment of making contact*. This mechanism is an implementation detail, which we will derive in our implementation steps. For now we only assume that agents can make contact with each other somehow.

The *parallel* strategy matches the semantics of the agent-based SIR model due to the underlying roots in the System Dynamics approach. As discussed already in Chapter 3.2, in the parallel update-strategy, the agents act conceptually all at the same time in lock-step. This implies that they observe the same environment state during a time-step and actions of an agent are only visible in the next time-step - they are isolated from each other. As will become apparent, FP can be used to enforce the correct application of this strategy already on the compile-time level.

We start by defining the SIR states as ADT and our agents as signal functions (SF) which receive the SIR states of all agents form the previous step as input and outputs the current SIR state of the agent. This definition, and the fact that Yampa is not monadic, guarantees already at compile, that the agents are isolated from each other, enforcing the *parallel* lock-step semantics of the model.

```
data SIRState = Susceptible | Infected | Recovered

type SIRAgent = SF [SIRState] SIRState

sirAgent :: RandomGen g => g -> SIRState -> SIRAgent
sirAgent g Susceptible = susceptibleAgent g
sirAgent g Infected    = infectedAgent g
sirAgent _ Recovered   = recoveredAgent
```

Depending on the initial state we return the corresponding behaviour. Note that we are passing a random-number generator instead of running in the Random Monad because signal functions as implemented in Yampa are not capable of being monadic.

We see that the recovered agent ignores the random-number generator because a recovered agent does nothing, stays immune forever and can not get infected again in this model. Thus a recovered agent is a consuming state from which there is no escape, it simply acts as a sink which returns constantly *Recovered*:

```
recoveredAgent :: SIRAgent
recoveredAgent = arr (const Recovered)
```

Next, we implement the behaviour of a susceptible agent. It makes contact *on average* with β other random agents. For every *infected* agent it gets into contact with, it becomes infected with a probability of γ. If an infection happens, it makes the transition to the *Infected* state. To make contact, it gets fed the states of all agents in the system from the previous time-step, so it can draw random contacts - this is one, very naive way of implementing the interactions between agents.

Thus a susceptible agent behaves as susceptible until it becomes infected. Upon infection an *Event* is returned, which results in switching into the *infectedAgent* SF, which causes the agent to behave as an infected agent from that moment on. When an infection event occurs we change the behaviour of an agent using the Yampa combinator *switch*, which is quite elegant and expressive as it makes the change of behaviour at the occurrence of an event explicit. Note that to make contact *on average*, we use Yampas *occasionally* function which requires us to carefully select the right Δt for sampling the system as will be shown in results.

Note the use of $iPre :: a \rightarrow SF\ a\ a$, which delays the input signal by one sample, taking an initial value for the output at time zero. The reason for it is that we need to delay the transition from susceptible to infected by one step due to the semantics of the *switch* combinator: whenever the switching event occurs, the signal function into which is switched will be run at the time of the event occurrence. This means that a susceptible agent could make a transition to recovered within one time-step, which we want to prevent, because the semantics should be that only one state-transition can happen per time-step.

```
susceptibleAgent :: RandomGen g => g -> SIRAgent
susceptibleAgent g
    = switch
      -- delay switching by 1 step to prevent against transition
      -- from Susceptible to Recovered within one time-step
      (susceptible g >>> iPre (Susceptible, NoEvent))
      (const (infectedAgent g))
  where
    susceptible :: RandomGen g => g -> SF [SIRState] (SIRState, Event ())
    susceptible g = proc as -> do
      makeContact <- occasionally g (1 / contactRate) () -< ()
      if isEvent makeContact
        then (do
          -- draw random element from the list
          a <- drawRandomElemSF g -< as
          case a of
            Infected -> do
              -- returns True with given probability
              i <- randomBoolSF g infectivity -< ()
              if i
                then returnA -< (Infected, Event ())
                else returnA -< (Susceptible, NoEvent)
            _        -> returnA -< (Susceptible, NoEvent))
        else returnA -< (Susceptible, NoEvent)
```

To deal with randomness in an FRP way, we implemented additional signal functions built on the *noiseR* function provided by Yampa. This is an example for the stream character and statefulness of a signal function as it allows to keep track of the changed random-number generator internally through the use of continuations and closures. Here we provide the implementation of *randomBoolSF*. *drawRandomElemSF* works similar but takes a list as input and returns a randomly chosen element from it:

```
randomBoolSF :: RandomGen g => g -> Double -> SF () Bool
randomBoolSF g p = proc _ -> do
```

```
  r <- noiseR ((0, 1) :: (Double, Double)) g -< ()
  returnA -< (r <= p)
```

An infected agent recovers *on average* after δ time units. This is implemented by drawing the duration from an exponential distribution [20] with $\lambda = \frac{1}{\delta}$ and making the transition to the *Recovered* state after this duration. Thus the infected agent behaves as infected until it recovers, on average after the illness duration, after which it behaves as a recovered agent by switching into *recoveredAgent*. As in the case of the susceptible agent, we use the *occasionally* function to generate the event when the agent recovers. Note that the infected agent ignores the states of the other agents as its behaviour is completely independent of them.

```
infectedAgent :: RandomGen g => g -> SIRAgent
infectedAgent g
    = switch
      -- delay switching by 1 step
      (infected >>> iPre (Infected, NoEvent))
      (const recoveredAgent)
  where
    infected :: SF [SIRState] (SIRState, Event ())
    infected = proc _ -> do
      recEvt <- occasionally g illnessDuration () -< ()
      let a = event Infected (const Recovered) recEvt
      returnA -< (a, recEvt)
```

For running the simulation we use Yampas function *embed*:

```
runSimulation :: RandomGen g => g -> Time -> DTime -> [SIRState] -> [[SIRState]]
runSimulation g t dt as
    = embed (stepSimulation sfs as) ((), dts)
  where
    steps     = floor (t / dt)
    dts       = replicate steps (dt, Nothing)
    n         = length as
    (rngs, _) = rngSplits g n [] -- unique rngs for each agent
    sfs       = zipWith sirAgent rngs as
```

What we need to implement next is a closed feedback-loop - the heart of every agent-based simulation. Fortunately, [111, 37] discusses implementing this in Yampa. The function *stepSimulation* is an implementation of such a closed feedback-loop. It takes the current signal functions and states of all agents, runs them all in parallel and returns this step's new agent states. Note the use of *notYet*, which is required to delay switching by one step to break a potentially infinite recursive switching. This is necessary because we are recursively switching back into the *stepSimulation*, which would result in the immediate evaluation of the next step, overriding the output of the current step, recursively switching back into *stepSimulation* and so on. The combinator *notYet* breaks this by delaying the switching event by one step.

```
stepSimulation :: [SIRAgent] -> [SIRState] -> SF () [SIRState]
stepSimulation sfs as =
```

```
    dpSwitch
      -- feeding the agent states to each SF
      (\_ sfs' -> (map (\sf -> (as, sf)) sfs'))
      -- the signal functions
      sfs
      -- switching event, delay by one step to prevent
      -- infinite recursion
      (switchingEvt >>> notYet)
      -- recursively switch back into stepSimulation
      stepSimulation
  where
    switchingEvt :: SF ((), [SIRState]) (Event [SIRState])
    switchingEvt = arr (\ (_, newAs) -> Event newAs)
```

Yampa provides the *dpSwitch* combinator for running signal functions in parallel, which has the following type-signature:

```
dpSwitch :: Functor col
         -- routing function
         => (forall sf. a -> col sf -> col (b, sf))
         -- SF collection
         -> col (SF b c)
         -- SF generating switching event
         -> SF (a, col c) (Event d)
         -- continuation to invoke upon event
         -> (col (SF b c) -> d -> SF a (col c))
         -> SF a (col c)
```

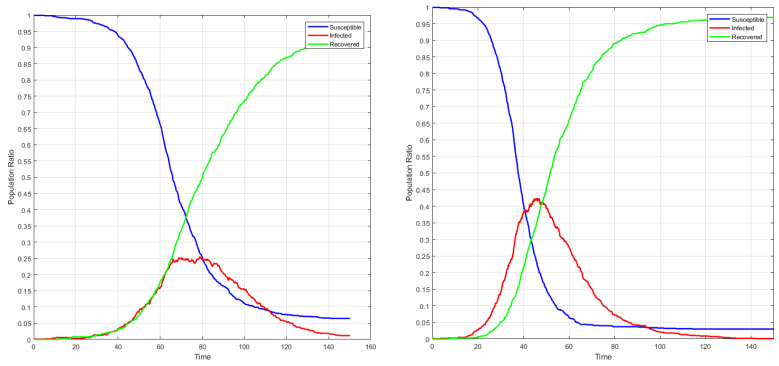
Its first argument is the pairing-function, which pairs up the input to the signal functions - it has to preserve the structure of the signal function collection. The second argument is the collection of signal functions to run. The third argument is a signal function generating the switching event. The last argument is a function, which generates the continuation after the switching event has occurred. *dpSwitch* returns a new signal function, which runs all the signal functions in parallel and switches into the continuation when the switching event occurs.

Conceptually, *dpSwitch* allows us to recursively switch back into the *stepSimulation* with the continuations and new states of all the agents after they were run in parallel.

4.1.1 Results

The dynamics generated by this step can be seen in Figure 4.1.

By following the FRP approach we assume a continuous flow of time, which means that we need to select a *correct* Δt, otherwise we would end up with wrong dynamics. The selection of a correct Δt depends in our case on *occasionally* in the *susceptible* behaviour, which randomly generates an event on average with *contact rate* following the exponential distribution. To arrive at the correct dynamics, this requires us to sample *occasionally*, and thus the whole system, with small enough Δt which matches the frequency of events generated by *contact rate*. If we choose a too large Δt, we loose events, which will result in wrong



(a) $\Delta t = 0.1$ (b) $\Delta t = 0.01$

Figure 4.1: FRP simulation of agent-based SIR showing the influence of different Δt. Population size of 1,000 with contact rate $\beta = \frac{1}{5}$, infection probability $\gamma = 0.05$, illness duration $\delta = 15$ with initially 1 infected agent. Simulation run for 150 time-steps with respective Δt.

dynamics as can be seen in Figure 4.1a. This issue is known as under-sampling and is described in Figure 4.2.

For tackling this issue we have three options. The first one is to use a smaller Δt as can be seen in 4.1b, which results in the whole system being sampled more often, thus reducing performance. The second option is to step the simulation with $\Delta t = 1$ and in each step, instead of using *occasionally*, to make a number of contacts drawn from the exponential distribution. Note that if we follow this option, we abandon the time-driven approach altogether because we don't abstract away from Δt and violate the fundamental abstraction of FRP which assumes that time is continuous and signal functions are running conceptually infinitely fast and infinitely often [165]. We will come back to this approach in the even-driven approach to ABS in Chapter 5.2. This leaves us with the third option to implement super-sampling and apply it to *occasionally*, which allows us then to run the whole simulation with $\Delta t = 1.0$ and only sample the *occasionally* function with a much higher frequency.

In Yampa there exists a function *embed* which allows to run a given signal-function with provided Δt but the problem is that this function does not really help because it does not return a signal-function. What we need is a signal-function which takes the number of super-samples n, the signal-function sf to sample and returns a new signal-function which performs super-sampling on it. We provide a full implementation of such a function, which also gives an insight into how signal functions are implemented in Yampa:

```
import FRP.Yampa.InternalCore

-- SF is the signal-function defined for time t = 0 and returns
-- a continuation of type SF' which is the signal-function
```

(a) Under-sampling

(b) Super-sampling

Figure 4.2: A visual explanation of under-sampling and super-sampling. The black dots represent the time-steps of the simulation. The red dots represent virtual events which occur at specific points in continuous time. In the case of under-sampling, 3 events occur in between the two time steps but *occasionally* only captures the first one. By increasing the sampling frequency either through a smaller Δt or super-sampling all 3 events can be captured.

```haskell
-- defined for t > 0: it receives an additional time-delta
-- data SF a b  = SF { sfTF :: a -> (SF' a b, b) }
-- data SF' a b = DTime -> a -> (SF' a b, b)

superSampling :: Int -> SF a b -> SF a [b]
superSampling n sf0 = SF { sfTF = tf0 }
  where
    -- no supersampling at time 0
    tf0 :: a -> (SF' a b, [b])
    tf0 a0 = (tfCont, [b0])
      where
        (sf', b0) = sfTF sf0 a0 -- running a SF
        tfCont    = superSamplingAux sf'

    superSamplingAux :: SF' a [b]
    superSamplingAux sf' = SF' tf
      where
            tf0 :: DTime -> a -> (SF' a b, [b])
        tf dt a = (tf', bs)
          where
            (sf'', bs) = superSampleRun n dt sf' a
            tf'        = superSamplingAux sf''

    superSampleRun :: Int -> DTime -> SF' a b -> a -> (SF' a b, [b])
    superSampleRun n dt sf a
        | n <= 1    = superSampleMulti 1 dt sf a []
        | otherwise = (sf', reverse bs)  -- reverse due to accumulator
      where
        superDt = dt / fromIntegral n
        (sf', bs) = superSampleMulti n superDt sf a []

    superSampleMulti :: Int -> DTime -> SF' a b -> a -> [b] -> (SF' a b, [b])
    superSampleMulti 0 _ sf _ acc  = (sf, acc)
    superSampleMulti n dt sf a acc = superSampleMulti (n-1) dt sf' a (b:acc)
      where
        (sf', b) = sfTF' sf dt a -- running a SF'
```

It evaluates the *SF* argument for n times, each with $\Delta t = \frac{\Delta t}{n}$ and the

same input argument a for all n evaluations. At time 0 no super-sampling is performed and just a single output of the *SF* argument is calculated. A list of b is returned with length of n containing the result of the n evaluations of the *SF* argument. If 0 or less super samples are requested exactly one is calculated. We could then wrap the occasionally function which would then generate a list of events.

4.1.2 Discussion

We can conclude that our first step already introduced most of the fundamental concepts of ABS:

- Time - the simulation occurs over virtual time which is modelled explicitly, divided into *fixed* Δt, where at each step all agents are executed.
- Agents - we implement each agent as an individual, with the behaviour depending on its state. It is clear to see that agents behave as signals: when the system is sampled with $\Delta t = 0$ then their behaviour will stay constant and won't change because it is completely determined by the flow of time.
- Feedback - the output state of the agent in the current time-step t is the input state for the next time-step $t + \Delta t$.
- Environment - as environment we implicitly assume a fully-connected network (complete graph) where every agent 'knows' every other agent, including itself and thus can make contact with all of them.
- Stochasticity - it is an inherently stochastic simulation, which is indicated by the random-number generator and the usage of *occasionally*, *randomBoolSF* and *drawRandomElemSF*.
- Deterministic - repeated runs with the same initial random-number generator result in same dynamics. This may not come as a surprise but in Haskell we can guarantee that property statically already at compile time because our simulation runs *not* in the IO Monad. This guarantees that no external, uncontrollable sources of non-determinism can interfere with the simulation.
- Parallel, lock-step semantics - the simulation implements a *parallel* update-strategy where in each step the agents are run isolated in parallel and don't see the actions of the others until the next step.

Using FRP in the instance of Yampa results in a clear, expressive and robust implementation. State is implicitly encoded, depending on which signal function is active. By using explicit time-semantics with *occasionally* we can achieve extremely fine grained stochastics by sampling the system with small Δt: we are treating it as a truly continuous time-driven agent-based system.

A very severe problem, hard to find with testing but detectable with in-depth validation analysis, is the fact that in the *susceptible* agent the same random-number generator is used in *occasionally*, *drawRandomElemSF* and *randomBoolSF*. This means that all three stochastic functions, which should be independent from each other, are inherently correlated. This is something one wants to prevent under all circumstances in a simulation, as it can invalidate the dynamics on a very subtle level, and indeed we have tested the influence of the correlation in this example and it has an impact. We left this severe bug in for explanatory reasons, as it shows an example where functional programming actually encourages very subtle bugs if one is not careful. A possible but not very elegant solution would be to simply split the initial random-number generator in *sirAgent* three times (using one of the splited generators for the next split) and pass three random-number generators to *susceptible*. A much more elegant solution would be to use the Random Monad which is not possible because Yampa is not monadic.

So far we have an acceptable implementation of an agent-based SIR approach. What we are lacking at the moment is a general treatment of an environment and an elegant solution to the random number correlation. In the next step we make the transition to Monadic Stream Functions as introduced in Dunai [122], which allows FRP within a monadic context and gives us a way for an elegant solution to the random number correlation.

4.2 Second Step: Going Monadic

A part of the library Dunai is BearRiver, a wrapper which re-implements Yampa on top of Dunai, which should allow us to easily replace Yampa with MSFs. This will enable us to run arbitrary monadic computations in a signal function, solving our problem of correlated random numbers through the use of the Random Monad.

4.2.1 Identity Monad

We start by making the transition to BearRiver by simply replacing Yampas signal function by BearRivers', which is the same but takes an additional type parameter m, indicating the monadic context. If we replace this type-parameter with the Identity Monad, we should be able to keep the code exactly the same, because BearRiver re-implements all necessary functions we are using from Yampa. We simply re-define the agent signal function, introducing the monad stack our SIR implementation runs in:

```
type SIRMonad = Identity
type SIRAgent = SF SIRMonad [SIRState] SIRState
```

4.2.2 Random Monad

Using the Identity Monad does not gain us anything but it is a first step towards a more general solution. Our next step is to replace the Identity Monad by the Random Monad, which will allow us to run the whole simulation within the Random Monad with the full features of FRP, finally solving the problem of correlated random numbers in an elegant way. We start by re-defining the SIRMonad and SIRAgent:

```
type SIRMonad g = Rand g
type SIRAgent g = SF (SIRMonad g) [SIRState] SIRState
```

The question is now how to access this Random Monad functionality within the MSF context. For the function *occasionally*, there exists a monadic pendant *occasionallyM* which requires a MonadRandom type-class. Because we are now running within a MonadRandom instance we simply replace *occasionally* with *occasionallyM*.

```
occasionallyM :: MonadRandom m => Time -> b -> SF m a (Event b)
-- can be used through the use of arrM and lift
randomBoolM :: RandomGen g => Double -> Rand g Bool
-- this can be used directly as a SF with the arrow notation
drawRandomElemSF :: MonadRandom m => SF m [a] a
```

4.2.3 Discussion

Running in the Random Monad solved the problem of correlated random numbers and elegantly guarantees us that we won't have correlated stochastics as discussed in the previous section. In the next step we introduce the concept of an explicit discrete 2D environment.

4.3 Third Step: Adding an environment

So far we have implicitly assumed a fully connected network amongst agents, where each agent can see and 'knows' every other agent. This is a valid environment and in accordance with the System Dynamics inspired implementation of the SIR model but does not show the real advantage of ABS to situate agents within arbitrary environments. Often, agents are situated within a discrete 2D environment [49] which is simply a finite NxM grid with either a Moore or von Neumann neighbourhood (Figure 4.3). Agents are either static or can move freely around with cells allowing either single or multiple occupants.

We can directly map the SIR model to a discrete 2D environment by placing the agents on a corresponding 2D grid with an unrestricted neighbourhood. The behaviour of the agents is the same but they select their interactions directly from the shared read-only environment, which will be passed to the agents as input. This allows agents to read the states of all their neighbours, which tells them if a neighbour is infected or not. To show the benefit over the System

(a) von Neumann (b) Moore

Figure 4.3: Common neighbourhoods in discrete 2D environments of Agent-Based Simulation.

Dynamics approach and for purposes of a more interesting approach, we restrict the neighbourhood to Moore (Figure 4.3b).

We also implemented this spatial approach in Java using the well known ABS library RePast [112], to have a comparison with a state of the art approach and came to the same results as shown in Figure 4.4. This supports, that our pure functional approach can produce such results as well and compares positively to the state of the art in the ABS field.

4.3.1 Implementation

We start by defining the discrete 2D environment for which we use an indexed two dimensional array. Each cell stores the agent state of the last time-step, thus we use the *SIRState* as type for our array data. Also, we re-define the agent signal function to take the structured environment *SIREnv* as input instead of the list of all agents as in our previous approach. As output we keep the *SIRState*, which is the state the agent is currently in. Also we run in the Random Monad as introduced before to avoid the random number correlation.

```
type Disc2dCoord = (Int, Int)
type SIREnv      = Array Disc2dCoord SIRState

type SIRAgent g  = SF (Rand g) SIREnv SIRState
```

Note that the environment is not returned as output because the agents do not directly manipulate the environment but only read from it. Again, this enforces the semantics of the *parallel* update-strategy through the types where the agents can only see the previous state of the environment and see the actions of other agents reflected in the environment only in the next step.

Note that we could have chosen to use a StateT transformer with the *SIREnv* as state, instead of passing it as input, with the agents then able to arbitrarily read/write, but this would have violated the semantics of our model because actions of agents would have become visible within the same time-step.

The implementation of the susceptible, infected and recovered agents are almost the same with only the neighbour querying now slightly different.

Stepping the simulation needs a new approach because in each step we need to collect the agent outputs and update the environment for the next next

step. For this we implemented a separate MSF, which receives the coordinates for every agent to be able to update the state in the environment after the agent was run. Note that we need use *mapM* to run the agents because we are running now in the context of the Random Monad. This has the consequence that the agents are in fact run sequentially one after the other but because they cannot see the other agents actions nor observe changes in the shared read-only environment, it is *conceptually* a *parallel* update-strategy where agents run in lock-step, isolated from each other at conceptually the same time.

```
simulationStep :: RandomGen g => [(SIRAgent g, Disc2dCoord)]
               -> SIREnv -> SF (Rand g) () SIREnv
simulationStep sfsCoords env = MSF (\_ -> do
  let (sfs, coords) = unzip sfsCoords
  -- run agents sequentially but with shared, read-only environment
  ret <- mapM (`unMSF` env) sfs
  -- construct new environment from all agent outputs for next step
  let (as, sfs') = unzip ret
      env' = foldr (\ (a, coord) envAcc -> updateCell coord a envAcc)
                env (zip as coords)

      sfsCoords' = zip sfs' coords
      cont       = simulationStep sfsCoords' env'
  return (env', cont))

updateCell :: Disc2dCoord -> SIRState -> SIREnv -> SIREnv
```

4.3.2 Results

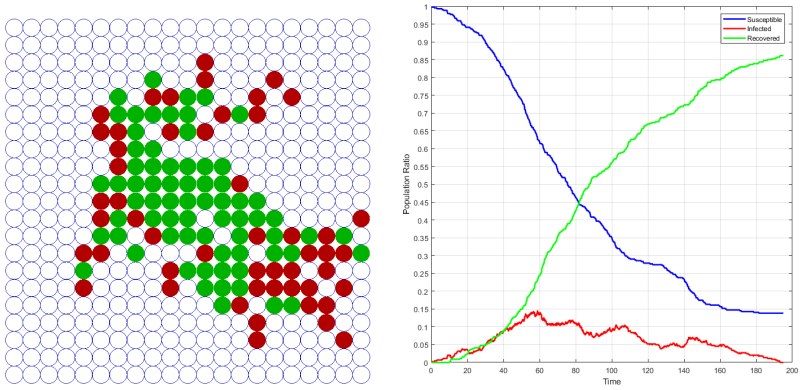
We implemented rendering of the environments using the gloss library which allows us to cycle arbitrarily through the steps and inspect the spreading of the disease over time visually as seen in Figure 4.4.

Note that the dynamics of the spatial SIR simulation, which are seen in Figure 4.4b look quite different from the reference dynamics of Figure 2.2. This is due to a much more restricted neighbourhood which results in far fewer infected agents at a time and a lower number of recovered agents at the end of the epidemic, meaning that fewer agents got infected overall.

4.3.3 Discussion

By introducing a structured environment with a Moore neighbourhood, we showed the ABS ability to place the heterogeneous agents in a generic environment, which is the fundamental advantage of an agent-based approach over other simulation methodologies and allows us to simulate much more realistic scenarios.

Note, that an environment is not restricted to be a discrete 2D grid and can be anything from a continuous N-dimensional space to a complex network - one only needs to change the type of the environment and agent input and provide corresponding neighbourhood querying functions.



(a) Environment at $t = 50$ (b) Dynamics over time

Figure 4.4: Simulating the agent-based SIR model on a 21x21 2D grid with Moore neighbourhood (Figure 4.3b), a single infected agent at the center and same SIR parameters as in Figure 2.2. Simulation run until $t = 200$ with fixed $\Delta t = 0.01$. Last infected agent recovers around $t = 194$. The susceptible agents are rendered as blue hollow circles for better contrast.

4.4 Discussion

Our FRP based approach is different from traditional approaches in the ABS community. First it builds on the already quite powerful FRP paradigm. Second, due to our continuous time approach, it forces one to think properly of time-semantics of the model and how small Δt should be. Third it requires one to think about agent interactions in a new way instead of being just method-calls.

4.4.1 Static guarantees

Because no part of the simulation runs in the IO Monad and we do not use *unsafePerformIO* we can rule out a serious class of bugs caused by implicit data-dependencies and side-effects, which can occur in traditional imperative implementations.

Also we can statically guarantee the reproducibility of the simulation, which means that repeated runs with the same initial conditions are guaranteed to result in the same dynamics. Although we allow side-effects within agents, we restrict them to only the Random Monad in a controlled, deterministic way and never use the IO Monad, which guarantees the absence of non-deterministic side effects within the agents and other parts of the simulation.

Determinism is also ensured by fixing the Δt and not making it dependent on the performance of e.g. a rendering-loop or other system-dependent sources of non-determinism as described by [123]. Also by using FRP we gain all the

benefits from it and can use research on testing, debugging and exploring FRP systems [123, 120].

Also we showed how to implement the *parallel* update-strategy [150] in a way that the correct semantics are enforced and guaranteed already at compile time through the types. This is not possible in traditional imperative implementations and poses another unique benefit over the use of functional programming in ABS.

The result of using FRP allows expressing continuous time-semantics in a very clear, compositional and declarative way, abstracting away the low-level details of time-stepping and progress of time within an agent.

Our approach can guarantee reproducibility already at compile time, which means that repeated runs of the simulation with the same initial conditions will always result in the same dynamics, something highly desirable in simulation in general. This can only be achieved through purity, which guarantees the absence of implicit side-effects, which allows to rule out non-deterministic influences at compile time through the strong static type system, something not possible with traditional object-oriented approaches. Further, through purity and the strong static type system, we can rule out important classes of run-time bugs e.g. related to dynamic typing, and the lack of implicit data-dependencies which are common in traditional imperative object-oriented approaches.

Using pure functional programming, we can enforce the correct semantics of agent execution through types where we demonstrate that this allows us to have both, sequential monadic behaviour, and agents acting *conceptually* at the same time in lock-step, something not possible using traditional object-oriented approaches.

4.4.2 Performance

Currently, the performance our approach does not come close to imperative implementations. We compared the performance of the time-driven SIR as presented in Section 4.3 to an implementation in Java using the ABS library RePast [112]. We ran the simulation until $t = 100$ on a 51x51 (2,601 agents) with $\Delta t = 0.1$ (unknown in RePast) and averaged 8 runs. The performance results make the lack of speed of our approach quite clear: the pure functional approach needs around 72.5 seconds whereas the Java RePast version just 10.8 seconds on our machine to arrive at $t = 100$. It must be mentioned, that RePast does implement an event-driven approach to ABS, which can be much more performant [108] than a time-driven one as ours, so the comparison is not completely valid.

As a remedy we compared a time-driven SIR implementation we did in Java to the pure functional implementations of Chapter 4.1. In the Java implementations we tried to follow conceptually similar approaches to the pure functional implementations but obviously that is not possible for every aspect. For example, we are not using any reactive programming library but we follow a similar time-sampling approach. We run for 150 time-steps with 1,000 susceptible and 1 infected agent, $\beta = 5$, $\gamma = 0.05$, $\delta = 15$ and $\delta t = 0.01$. Further, we fixed the

random-number generators to guarantee identical dynamics in every run and averaged 8 runs. The time-driven Java implementation averages at a performance of 0.5 seconds, compared to 27.6 seconds in Haskell. The implementation of 4.3 with the same configuration using a 10x10 environment with no neighbourhood restrictions averages at 19 seconds.

We expect a substantial performance improvement when switching to an event-driven approach [108] in the next Chapter 5.1. Further, the performance issue will be addressed more in-depth in the chapters on parallelism 7 and concurrency 8.

4.4.3 Drawbacks

Despite the strengths and benefits we get by leveraging on FRP, there are errors that are not raised at compile time, e.g. we can still have infinite loops and run-time errors. This was for example investigated in [136] where the authors use dependent types to avoid some run-time errors in FRP. We suggest that one could go further and develop a domain specific type system for FRP that makes the FRP based ABS more predictable and that would support further mathematical analysis of its properties. Furthermore, moving to dependent types would pose a unique benefit over the traditional object-oriented approach and should allow us to express and guarantee even more properties at compile time. We leave this for further research.

In our pure functional approach, agent identity is not as clear as in traditional object-oriented programming, where there is a quite clear concept of object-identity through the encapsulation of data and methods. Signal functions don't offer this strong identity and one needs to build additional identity mechanisms on top e.g. when sending messages to specific agents.

We can conclude that the main difficulty of a pure functional approach evolves around the communication and interaction between agents, which is a direct consequence of the issue with agent identity. Agent interaction is straightforward in object-oriented programming, where it is achieved using method-calls mutating the internal state of the agent, but that comes at the cost of a new class of bugs due to implicit data flow. In pure functional programming these data flows are explicit but our current approach of feeding back the states of all agents as inputs is not very general. We address this problem in the next chapter.

Chapter 5

Pure Functional Event-Driven ABS

In this chapter we build on the previous discussion of update-strategies in Chapter 3 and the implementation techniques presented in the time-driven approach of Chapter 4 to develop concepts for event-driven ABS in a pure functional way.

In event-driven ABS [108], the simulation is advanced through events: agents and the environment schedule events into the future and react to incoming events scheduled by themselves, other agents, the environment or the simulation kernel. Time is discrete in this approach: it advances step-wise from event to event, where each event has an associated time-stamp, which indicates the virtual simulation time when it is scheduled. This implies that time could stay constant e.g. when an event is scheduled with a time-delay of 0 the virtual simulation time does not advance. Because agents can adopt and change their state and behaviour when processing an event, this means that even if time does not advance, agents can change. This non-signal behaviour is the fundamental difference to the time-driven approach in Chapter 4. Further, we exploit this mechanism to implement direct agent-interactions in pure functional ABS as discussed in the Sugarscape use-case below.

The event-driven approach makes the simulation kernel technically closely related to a Discrete Event Simulation (DES) [167]. Due to the necessity of imposing a correct ordering of events in this type of ABS, we need to step it event by event, with the *sequential* update-strategy being the only feasible one for this type of ABS. Note that there exists also Parallel DES (PDES) [56], which processes events in parallel and deals with inconsistencies by reverting to consistent states - we hypothesize that a pure functional approach could be beneficial in such an approach due to persistent data-structures and explicit handling of side-effects but we leave this for further research.

We use the Sugarscape model to develop pure functional concepts for event-

driven ABS [1]. We chose this model for the following reasons: it is quite well known in the ABS community; it was highly influential in sparking the interest in ABS; it is quite complex with non-trivial agent-interactions; the original implementation was done in Object Pascal and C with about 20.000 lines of code which includes GUI, graphs and plotting, where they used Object Pascal for programming the agents and C for low-level graphics [12]; the authors explicitly advocate OOP as a good fit to ABS which begged the question whether and how well a pure functional implementation is possible. The Sugarscape model is not a classic event-driven model: in it the agents do schedule events but they don't do this into the future - events in Sugarscape don't have associated time-stamps. Still the underlying concepts are the same as in event-driven ABS and it is trivial to add time-stamps as we will show in an additional section where we implement an event-driven implementation of the previously introduced agent-based SIR model, moving towards a real event-driven ABS with DES character.

5.1 Implementation Concepts

TODO REFINE / REWORK / REWRITE CHAPTER - IMPORTANT: follow same step-by-step approach as in time-driven approach: make clear we are using sequential iteration strategy, then add environment on top of rand, then scheduling of events, adding of local encapsulated state, using a transformer approach, then switch to tagless final, then finally introduce sync agent-interactions which are possible through tagless final

- IMPORTANT!!! i got the intuition that using the event-driven SIR implementation to introduce the basic concepts here is of more value than jumping straight into the highly complex sugarscape. The reasons: the SIR is already covered in the chapter before and thus well known; i use the event-driven in the property-based chapter (a lot) but have not really discussed it on a technical level; i can really show all concepts with full code, in sugarscape it is so much that we cannot do this. Still I want to discuss Sugarscape as well in-depth as it demonstrates that we can implement a highly complex simulation in Haskell as well. I just need to fit it better into the overall narrative: yes discuss some technical details but also focus on the more software-engineering part

- motivate each step carefully step-by-step, ultimately we derive immutable, pure functional objects here which we became aware of only after we properly reflected on it in the conclusions. this is no coincidence: the deeper idea behind objects (exchange of messages with shared nothing semantics with internal immutable state) seems indeed to be a good approach to ABS. indeed, we could also implement a sugarscape completely different with pure functions and data-structures over which we iterate: this is then a completely data-centric approach without any encapsulation and abstraction: this is what we do NOT want here? encapsulation and abstraction is good, otherwise we have a blob of mutable data with a data-flow which is difficult to reason about, even if it

[1] The code of all steps can be accessed freely from: `https://github.com/thalerjonathan/phd/tree/master/public/towards/SugarScape/sequential`

is pure functional programming. In ACE this is less a problem, as the gintis case and the zero intelligence implementations show: agents there can be really implemented using a simple newtype or data-structures with pure functions (and a few MonadRandom ones), why? because there the model is much more about data, data-representation and data-flow than interaction of agents like in the sugarscape. This is also a bit the case in the previous chapter on time-driven ABS where the agents act continously over time, reflecting a much more data-flow centric approach than an interaction-centric one. In this chapter the interaction move into the center and we show how to achieve that in ABS: how we can represent interacting agents in a pure functional way. The reason why we named it event-driven is that events or messages are the heart of interactions between agents; after all it is no coincidence that in OO terminology method calls are also synonymous with sending a message to an object - can we follow a cleaner Tagless Final approach like i prototyped in SIR? this allows easier extensibility in both dimensions: adding new operations (what agents are allowed to do) and new interpreter (pure functional, STM concurrency, IO concurrency). I will learn a great deal about this, it will be a strong selling point and it might event allow to implement synchronous interactions?? - use MTL instead of fully expanded stack! e.g. MonadRandom instead of Rand - In the time-driven approach we already introduced the use of effectful SignalFunctions: Monadic Stream Functions (MSF), where we only used a simple Rand effect to draw random number streams. Due to the much greater complexity of the Sugarscape we will want to make use of a whole layer of effects. To manage them in a clean way we follow a so called *Tagess Final* approach [95]. The idea relies heavily on defining operations using type-classes and the implementing concrete instances for them which act as interpreters. The main benefit is that a Tagless Final approach is extensible in two dimensions: we can add new interpreters to existing data-types and we can add new operations. Ultimately, this allows us to separate specification from implementation, following a similar approach as Free Monads (see future research) without the problems of their performance penalty. - we can write combinators which encapsulate all the continuation plumbing so it looks in the end very similar to a method call: shortly discuss and show that in Sugarscape. implement sync-interaction combinator: it becomes clear in the type of the function what is going on

In the next sections we derive implementation concepts of pure functional event-driven ABS. Due to the complexity of the Sugarscape model we don't provide a full implementation but only present concepts derived from our implementation and present small parts of the Sugarscape implementation when necessary.

5.1.1 Agent Representation

We follow the same approach as in the time-driven approach of Chapter 4.2 and use an MSF to define our agent due to the following requirements:

- As in the time-driven approach, we need a random number stream within

our agents, for which we will make use of the *Rand* monad.

- In the Sugarscape, the agents act on an environment which they both read *and* write. We will make use of the *State* monad for this functionality.
- The agents state in the Sugarscape model is much more complex than in the time-driven example where it was implicit. In this approach the agents have an explicit data-structure which they can mutate whenever they are acting. We will make use of the *State* monad for this functionality.
- For synchronous and one-way agent-interactions, agents send messages to other agents. This is completely different from the time-driven approach where no direct agent-interactions in form of messages where possible because agents were all acting at the same time and synchronous agent-interactions would violate that principle. We will make use of the *Writer* monad for this functionality.
- Due to the agent-interaction through messaging we need a clearly defined concept of agent identity, which is immutable for each agent and fixed at agent-creation time. At the same time we also need to generate new agent identities e.g. when an agent needs to create a new born from mating action. Further we need to access the read-only model configuration which defines if e.g. trading is turned on or off. We will make use of the *Reader* and *State* monad for this functionality.

The interface of an agent changes now substantially with very different inputs and outputs due to the fundamental different model and ABS type. Because we are dealing with events now, it makes very much sense to define the input-type of an agent as the event-type: this indicates that an agent always needs an event to run, to which it will react. As output we need a much richer structure than simply the current state the agent is in as in the time-driven approach: we need to be able to communicate to the simulation kernel whether the agent should be removed from the simulation, what new agents this agent wants to create and what messages it sends to other agents. Additionally we need to communicate the observable properties of an agent to the simulation kernel for visualisation purposes. We will show below how to conveniently construct such an output in a monadic way through the *Writer* monad. Note that many additional inputs and outputs are implicitly covered by the monadic context as will be shown below, e.g. we could also pass the environment as input and returning it as output instead providing it through a *State* monad but the latter is much more convenient to program with.

5.1.1.1 A generic MSF for event-driven ABS

We start with defining the basic types for a general event-driven agent. Besides the obligatory Time and Δt which are defined in this case as *Int* we define an *AgentId* as *Integer* for uniquely identifying agents in the process of messaging. Further an event type is defined which is either a *Tick* with a given Δt or a

DomainEvent from a given sender with the given event where the type of the actual *DomainEvent* is generic. As already mentioned we need a way of generating new agent identities which happens through the *ABSState* data structure which holds the next agent-id plus the current virtual simulation time so that agents don't need to keep track of it themselves. Now we can define the initial *AgentT* monad-transformer for which we start with a *StateT* and the previously defined *ABSState*.

Finally we define the type of the Agent MSF as a simple monadic stream function (MSF) with the monadic context *AgentT* and the *ABSEvent* as input. The output is the previously mentioned structure and the observable properties of the agent. The Agent MSF is parametrised by m indicating the type of (additional) monadic context, e indicating the type of the *DomainEvent* and o indicating the type of the observable properties. These types are highly polymorphic and are applicable to a wide range of event-driven ABS models. Note that no explicit type of an environment is used because some models rather omit an explicit environment and have it implicitly encoded in the model itself e.g. a fully connected network of agent-neighbourhoods as in the agent-based SIR model in Chapter 4.1. Further, we also don't provide random-number generator functionality on the type-level at that point because concrete models might opt for a different approach to randomness e.g. providing their own random number generator through a monad-transformer or omitting it altogether. All this optional behaviour is possible because the monadic context of the agents MSF is a transformer which allows to add arbitrary number of layers of behaviour as we will see below: we are polymorphic in the side-effects, which is only possible in a pure functional language like Haskell and can't be achieved in the established OOP approaches to ABS.

```
type Time  = Int
type DTime = Int

type AgentId = Integer

data ABSEvent e = Tick DTime | DomainEvent AgentId e

data ABSState = ABSState
  { absNextId :: AgentId -- holds the next agent-id
  , absTime   :: Time    -- current simulation time
  }

type AgentT m       = StateT ABSState m
type AgentMSF m e o = MSF (AgentT m) (ABSEvent e) (AgentOut m e o, o)

-- definition of a new agent
data AgentDef m e o = AgentDef
  { adId      :: AgentId         -- unique agent-id
  , adSf      :: AgentMSF m e o  -- the agent behaviour function
  , adInitObs :: o               -- the value of the initial observable properties
  }

data AgentOut m e o = AgentOut
  { aoKill   :: Any              -- True if this agent should be removed
```

```
  , aoCreate :: [AgentDef m e o] -- a list of agents to create
  , aoEvents :: [(AgentId, e)]   -- a list of events (receiver, event)
  }
```

What is striking, and underlines the even-driven approach, is that we are using an MSF and not a monadic SF (Streamfunction) from Bearriver as we did in Chapter 4.2. This means that there is no inherent notion of a Δt available to the agent, which is precisely what we need in event-driven ABS. Time only advances through specific events, in this case the *Tick DTime* event.

5.1.1.2 Parametrising for Sugarscape

For our Sugarscape implementation, we need to parametrise the polymorphic types by concrete types for m, e and o. Further, we need access to a random-number stream and we want to make the unique agent-id, the environment and the model-configuration explicit in the types. We start with defining both the environment and model-configurations as new data-structures (see below) and the data-type for an individual agent-state and the observable properties of the agent. Note that we explicitly decided to use two different types for the agent-state and its observable properties - after all we could have used the type of the agent-state also as the type for its observable properties. With two different types we make the distinction between the (read/write) local agent-state and the (read-only) observable properties very clear. Also, it allows us to expose a much smaller subset of the agent-local state to the visualisation and export layer of the simulation. This gives us the ability to hide away agent-state fields, which are implementation detail or unimportant for visualisation and exporting purposes.

```
data SugEnvironment     = ...
data SugarScapeScenario = ...

data SugAgentState = SugAgentState
  { sugAgSugarMetab   :: Int
  , sugAgVision       :: Int
  , sugAgSugarLevel   :: Double
  , sugAgInitSugEndow :: Double
  , sugAgAge          :: Int
  , ...
  }

data SugAgentObservable = SugAgentObservable
  { sugObsSugMetab :: Int
  , sugObsVision   :: Int
  , sugObsSugLvl   :: Double
  , sugObsAge      :: Int
  ...
  }
```

As already mentioned, we can add additional behaviour through the monad transformer of the agents MSF. We use this to make the Sugarscape environment explicit in the types and add random number-functionality. We simply start out

with a *StateT* transformer for the Sugarscape environment, because the agent can read and write it and then terminate the transformer by adding the *Rand* monad for the random-number functionality. We then simply parametrise the existing monad transformer of *AgentMSF* with this additional transformer stack to arrive at the final type of the Sugarscapes agent MSF.

```
data SugEvent = ... -- all events of the sugarscape model

type SugAgentMonad g = StateT SugEnvironment (Rand g)
-- the sugarscape agent MSF with the monadic type expanding to:
-- AgentMSF (SugAgentMonad g)
-- =>
-- MSF (AgentT (SugAgentMonad g))
-- =>
-- MSF (StateT ABSState (SugAgentMonad g))
-- =>
-- MSF (StateT ABSState (StateT SugEnvironment (Rand g)))
type SugAgentMSF g = AgentMSF (SugAgentMonad g) SugEvent SugAgentObservable
```

Finally we define the type of the top-level agent-behaviour function. As already noted, we want to make the unique agent-id and the model-configuration explicit, so it will be passed as an argument to the function. Further we pass the initial agent state as an additional input. This function will then construct a corresponding initial MSF (see below) and returns it. Thus the intended behaviour is as follows: an agent is defined in terms of this top-level function, which will be passed to the simulation kernel (see below) which will in turn run this function to get the agents initial MSF which will then be run subsequently (see below).

```
type SugarScapeAgent g = SugarScapeScenario -> AgentId -> SugAgentState -> SugAgentMSF g
```

Now we have fully specified types for the Sugarscape agent. The types indicate very clearly the intention and the interface. What is of very importance is that we don't have any impure *IO* monadic context anywhere in our type-definitions and we can also guarantee that it won't get sneaked in: the transformer-stack of the agents MSF is terminated through the *Rand* monad - it is simply not possible to add other layers. In the next step we look at how the agent handles and send events - that is we are looking at an implementation of a *SugarScapeAgent* function.

5.1.1.3 Agent-Local abstractions

The top-level *SugarScapeAgent* function encapsulates the whole agent-behaviour, which is completely driven by events, passed in as input. We now look at how to define agent-local behaviour, which is hidden behind the *SugarScapeAgent* function-type: whereas the previously defined types are exposed to the whole simulation, the following deals with types and behaviour which is locally encapsulated and hidden from the simulation kernel. We want to achieve the following functionality, local to the agent: encapsulation of the agents' state

which should still be read/writeable, sending of events and read-only access to the agents unique id and the model configuration.

To implement the local encapsulation of the agents' state is straight forward with MSFs as they are continuations, which allow to capture local data using closures. Fortunately we don't need to implement the low-level plumbing, as dunai provides us with the a feedback function: *feedback :: Monad m ⇒ c → MSF m (a, c) (b, c) → MSF m a b*. It takes an initial value of type *c* and an MSF which takes in addition to its input *a* also the given type *c* and outputs in addition to type *b* also the type *c*, which clearly indicates the read/write property of type *c*. The function returns a new MSF which only operates on *a* as input and returns *b* as output by running the provided MSF and feeding back the *c* (with the initial *c* at the first call).

```
agentMsf :: RandomGen g => SugarScapeAgent g
agentMsf params aid s0 = feedback s0 (proc (evt, s) -> do ... )
```

Next we want to write a monadic function which handles our event. As already pointed out this function must be able to manipulate the agent-local state we just encapsulated through *feedback*, sending events and accessing the model configuration and the unique agent-id. Providing the local agent state is trivially done using the *State* monad. Providing the model configuration and the unique agent-id is trivially done using the *Reader* monad. For providing the event sending function we opted for the *Writer* monad: as shown above in the generic types, an agent outputs (amongst others) a list of events it wants to send to receivers. Thus we start with an empty initial list and provide functionality to append to this list - which is exactly what the *Writer* monad does: it allows to write to a data-type which implements the *Monoid* class. The lists in Haskell are instances of the *Monoid* class, thus this is covered for us already. Instead of only covering the event sending functionality with the *Writer* monad, we extend it to the whole *SugAgentOut* type which respective fields are instances of the *Monoid* class themselves thus writing an instance of the *Monoid* class for *SugAgentOut* is trivial. We thus define the following monad which is local to the agent and is only used *within AgentMSF*.

```
type SugAgentMonadT g = AgentT (SugAgentMonad g)
-- FULLY EXPANDS TO:
-- AgentT (SugAgentMonad g)
--  =>
-- AgentT (StateT SugEnvironment (Rand g))
--  =>
-- StateT ABSState (StateT SugEnvironment (Rand g))

type AgentLocalMonad g = WriterT (SugAgentOut g)
                           (ReaderT (SugarScapeScenario, AgentId)
                             (StateT SugAgentState (SugAgentMonadT g)))
-- FULLY EXPANDS TO (one step replacement of SugAgentMonadT):
-- WriterT (SugAgentOut g)
--  (ReaderT (SugarScapeScenario, AgentId)
--    (StateT SugAgentState
--      (StateT ABSState
```

```
--         (StateT SugEnvironment
--           (Rand g)))
```

Now we can define the MSF which handles an event. It has the *AgentLocalMonad* monadic context, takes an *ABSEvent* parametrised over *SugEvent* (thus it has also to handle *Tick*). What might come as a surprise is that it returns unit-type, implying that the results of handling an event are only visible as side-effects in the monad stack. This is intended. We could pass all arguments explicitly as input and/or output but that would complicate the handling code substantially, thus we opted for a monadic, imperative style handling of events.

```
type EventHandler g = MSF (AgentLocalMonad g) (ABSEvent SugEvent) ()
```

To run the handler, which has an extended monadic context within the *SugarScapeAgent* we make use of dunais functionality which provides functions to run MSFs with additional monadic layers within MSFs with less - similar to the *Control.Monad* approach. We use *runStateS*, *runReaderS* and *runWriterS* (*S* indicates the stream character) to run the *generalEventHandler*, providing the initial values for the respective monads: *s* for the *StateT*, *(params, aid)* for the *ReaderT* and the *evt* as the normal input to the event handler. Note that *WriterT* does not need an initial value, it will be provided through the *Monoid* instance of *AgentOut*.

```
agentMsf :: RandomGen g => SugarScapeAgent g
agentMsf params aid s0 = feedback s0 (proc (evt, s) -> do
  (s', (ao', _)) <- runStateS (runReaderS (runWriterS generalEventHandler)) -< (s, ((params, aid), evt))
  let obs = sugObservableFromState s
  returnA -< ((ao', obs), s'))

generalEventHandler :: RandomGen g => EventHandler g

sugObservableFromState :: SugAgentState -> SugAgentObservable
```

5.1.1.4 Handling and sending of Events

Now we can handle events on an agent-local level: we receive the events from the simulation kernel as input and run within a 6-layered monad transformer stack which is part global to the agent (controlled by the simulation kernel) and part local to the agent (controlled by the agent itself). The layers are the following (outer to inner):

1. WriterT (SugAgentOut g): *agent-local*, provides write-only functionality for constructing the agent-output for the simulation kernel which indicates whether to kill the agent, a list of new agents to create and a list of events to send to receiving agents.

2. ReaderT (SugarScapeScenario, AgentId): *agent-local*, provides the model configuration and unique agent-id read-only.

3. StateT SugAgentState: *agent-local*, provides the local agent state for reading and writing.

4. StateT ABSState: *global*, provides unique agent-ids for new agents and the current simulation time. The usage of a *StateT* is slightly flawed here because it provides too much power: the current simulation time should be read-only to the agent. Drawing the next agent-id involves reading the current id and writing the incremented value, thus technically it is a *StateT* but ideally we would like to hide the writing operation and only provide a *read-current-and-increment* operation. A possible solution would be to provide the current simulation time through a *ReaderT* and the new agent-id through a new monad which uses the *StateT* under the hood, like the *Rand* monad.
5. StateT SugEnvironment: *global*, provides the sugarscape environment which the agents can read and write.
6. Rand g: *global*, provides the random-number stream for all agents.

The event handler simply matches on the incoming events, extracts data and dispatches to respective handlers. What is crucial here to understand is that only the top level *agentMSF* and the *EventHandler* function are MSFs which simply dispatch to monadic functions, implementing the functionality in an imperative programming style. The main benefit of the MSFs are their continuation character, which allows to encapsulate local state. Further the dunai library adds a lot of additional functionality of composing MSFs and running different monadic context on top of each other. It even provides exception handling through MSFs with the *Maybe* type, thus programming with exceptions in ABS models can be done as well (we didn't make use of it, as the Sugarscape model simply does not specify any exception handling on the model level and there was also no opportunity to use exceptions from which to recover on a technical level - there are exceptions on a technical level but they are non-recoverable and should never occur at runtime, thus *error* is used, which terminates the simulation with an error message).

```
data SugEvent = MatingRequest AgentGender
              | MatingReply (Maybe (Double, Double, Int, Int, CultureTag, ImmuneSystem))
              ...

generalEventHandler :: RandomGen g => EventHandler g
generalEventHandler =
  continueWithAfter -- optionally switching the top event handler
    (proc evt ->
      case evt of
        Tick dt -> do
          mhdl <- arrM handleTick -< dt
          returnA -< ((), mhdl)

        (DomainEvent sender (MatingRequest otherGender)) -> do
          arrM (uncurry handleMatingRequest) -< (sender, otherGender)
          returnA -< ((), Nothing)
        ...)

handleTick :: RandomGen g => DTime -> AgentLocalMonad g (Maybe (EventHandler g))
handleMatingRequest :: AgentId -> AgentGender -> AgentLocalMonad g ()
```

Note the use of *continueWithAfter*, which is a customised version of the already known *switch* combinator, as used in Chapter 4.1. It allows to swap out the event-handler for a different one, which is the foundation for the synchronous agent-interactions, where it will be discussed more in-depth.

To see how an event handler works, we provide the implementation of *handleMatingRequest*. It is sent by an agent to its neighbours to request whether they want to mate with this agent. The handler receives the sender and the other agents gender (see *generalEventHandler*) and replies with *sendEventTo* which sends a *MatingReply* event back to the sender. The function *sendEventTo* operates on the *WriterT* to append (using *tell*) an event to the list of events this agent sends when handling this event. Note the use of *agentProperty*, which reads the value of a given field of the local agent state.

```
handleMatingRequest :: AgentId
                    -> AgentGender
                    -> AgentLocalMonad g ()
handleMatingRequest sender otherGender = do
  -- check if the agent is able to accept the mating request:
  -- fertile, wealthy enough, different gender
  accept <- acceptMatingRequest otherGender

  -- each parent provides half of its sugar-endowment for the new-born child
  acc <- if not accept
      then return Nothing
      else do
        sugLvl  <- agentProperty sugAgSugarLevel
        spiLvl  <- agentProperty sugAgSpiceLevel
        metab   <- agentProperty sugAgSugarMetab
        vision  <- agentProperty sugAgVision
        culTag  <- agentProperty sugAgCultureTag
        imSysGe <- agentProperty sugAgImSysGeno

        return Just (sugLvl / 2, spiLvl / 2, metab, vision, culTag, imSysGe)

  sendEventTo sender (MatingReply acc)
```

Next we look at how synchronous agent-interactions work - that is we look closer at the mating-mechanism which requires multiple synchronous interaction steps, which need to happen within the same simulation tick and both agents must not engage with other agents.

5.1.1.5 Synchronous Agent-Interactions

With the concepts introduced so far we can achieve already a lot in terms of agent-interactions: agents can react to incoming events, which are either the Tick-event advancing simulation time by one step or a message sent by another agent (or the agent itself). This is enough to implement simple one-directional asynchronous agent-interactions where one agent sends a message to another agent but does not await an answer within the same tick. This one-directional asynchronous interactions is used in the model to implement the passing of diseases, the paying back of debt, passing on wealth to children upon death - the agent simply sends a message and forgets about it.

Unfortunately this mechanism is not enough to implement the other agent-interactions in the Sugarscape model, which are structurally richer: they need to be synchronous. In the use-cases of mating, trading and lending two agents need to come to an agreement over multiple interactions steps within the same tick which need to be exclusive and synchronous. This means that an agent A initiates such a multi-step conversation with another agent B by sending an initial message to which agent B has to react by a reply to agent A who upon reception of the message, will pick up computation from that point and reply with a new message and so on. Both agents must not interact with other agents during this conversation to guarantee resource constraints, otherwise it would become quite difficult and cumbersome to ensure that agents don't spend more than they have when trading with multiple other agents at the same time. Also the initiating agent A must be able to pick up processing of its Tick event from the point where it started the conversation with agent B because sending a message always requires the handling of the current event to exit and hand the control back to the simulation kernel. See Figure 5.1 for a visualisation of the sequence of actions.

The way to implement this is to allow an agent to be able to change its internal event-handling state: to switch into different event-handlers, after having sent an event, to be able to react to the incoming reply in a specific way by encapsulating local state for the current synchronous interaction through closures and currying. Further by making use of continuations the agent can pick up the processing of the 'Tick' event after the synchronous agent-interaction has finished. Key to this is the function *continueWithAfter* which we already shortly introduced through *generalEventHandler*. This function takes an MSF which returns an output b and an optional MSF. If this optional Maybe MSF is Just then the *next* input is handled by this new MSF. In case no new MSF is returned (Nothing), the MSF will stay the same. This is a more specialised version of the *switch* combinator introduced in Chapter 2.3.3 in the way that it doesn't need an additional function to produce the actual MSF continuation. Note that the semantics are different though: whereas *continueWithAfter* only applies the new MSF in the *next* step, *switch* runs the new MSF immediately. The implementation of the function is as follows:

```
continueWithAfter :: Monad m => MSF m a (b, Maybe (MSF m a b)) -> MSF m a b
continueWithAfter msf = MSF (\a -> do
  ((b, msfCont), msf') <- unMSF msf a
  let msfNext = fromMaybe (continueWithAfter msf') msfCont
  return (b, msfNext))
```

We can now look at the Tick handling function. It returns a Maybe (EventHandler g) which if is Just will result in to a change of the top-level event handler through *continueWithAfter* as shown in *generalEventHandler* above. Note the use of continuations in the case of *agentMating, agentTrade, agentLoan*. All these functions return a Maybe (EventHandler g) because all of them can potentially result in synchronous agent-interactions which require to change the top-level event handler. When calling *agentDisease* we are passing a default

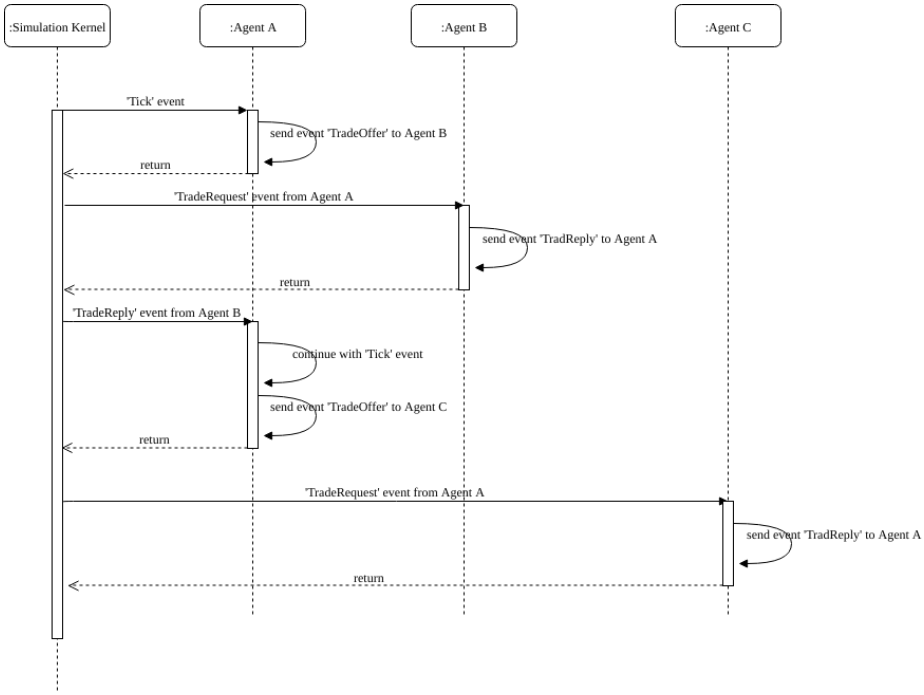


Figure 5.1: Sequence diagram of synchronous agent-interaction with the trading use-case. Upon the handling of the 'Tick' event, Agent A looks for trading partners and finds Agent B within its neighbourhood and sends a 'TradingOffer' message. Agent B replies to this message and Agent A continues with the trading algorithm by picking up where it has left the execution when sending the message to Agent B. After Agent A has finished the trading with Agent B, it turns to Agent C, where the same procedure follows and is thus not included fully in this diagram.

continuation which simply switches back into *generalEventHandler* to finish the processing of a Tick in an agent.

```
handleTick :: RandomGen g => DTime -> AgentLocalMonad g (Maybe (EventHandler g))
handleTick dt = do
  agentAgeing dt

  harvestAmount <- agentMove
  metabAmount   <- agentMetabolism
  agentPolute harvestAmount metabAmount

  ifThenElseM
    (starvedToDeath `orM` dieOfAge)
    (do
      agentDies agentMsf
      return Nothing)
    -- pass agentContAfterMating as continuation to pick up after mating
    -- synchronous conversations have finished
    (agentMating agentMsf agentContAfterMating)

-- after mating continue with cultural process and trading
agentContAfterMating :: RandomGen g => AgentLocalMonad g (Maybe (EventHandler g))
agentContAfterMating = do
    agentCultureProcess
    -- pass agentContAfterTrading as continuation to pick up after trading
    -- synchronous conversations have finished
    agentTrade agentContAfterTrading

-- after trading continue with lending and borrowing
agentContAfterTrading :: RandomGen g  => AgentLocalMonad g (Maybe (EventHandler g))
agentContAfterTrading = agentLoan agentContAfterLoan

-- after lending continue with diseases, which is the step in a Tick event
agentContAfterLoan :: RandomGen g => AgentLocalMonad g (Maybe (EventHandler g))
agentContAfterLoan = agentDisease defaultCont

-- safter diseases imply switch back into the general event handler
defaultCont :: RandomGen g => AgentLocalMonad g (Maybe (EventHandler g))
defaultCont = return (Just generalEventHandler)
```

5.1.2 Environment Representation

Environment representation is quite simpl, after we have solved the problem of how the agent can access it by using StateT. It is only a matter of selecting the right data-structure and writing domain-specific functions of the corresponding model to mutate the environment. Initially we used an indexed array from the *array* package. This data-structure has excellent read performance but in performance tests it was shown that it has serious performance and memory leak issues with updates, leading to allocation of about 40 MByte / second on our machine. Clearly this is unacceptable for simulation purposes, which often requires software to run for hours, and thus needs a constant memory consumption and must prevent even slowly linearly increasing memory usage under all costs. The solution was to switch to *IntMap* from the *containers* package as an underlying data-structure. We used the discrete 2d-coordinates to

map the environment cells to a unique index. This solved both the performance and memory leak issues completely.

5.1.2.1 Environment Behaviour

We must make a clear distinction between the environments data-structure and how agents access it and the environments behaviour. In the Sugarscape model, the behaviour of the environment is quite trivial: it simply regrows resources over time and diffuses pollution in case pollution is turned on. This behaviour is achieved by providing a pure function without any monadic context or MSF. This is not necessary because the environment how we implement it, does not encapsulate local state and it does not interact with agents through messages and vice versa. Thus a pure function which maps the environment to the environment is enough: $Time \rightarrow SugEnvironment \rightarrow SugEnvironment$. Further it also takes the current simulation time so it can implement seasons, where the speed of regrowth of resources is different in different regions and swaps after some time. This function is called in the simulation kernel after every Tick (see below).

Generally, one can distinguish between four different types of environments in ABS:

1. *Passive read-only* - implemented in Chapter 4.1, where the environment itself is not modelled as an active process and is static information, e.g. a list of neighbours, passed to each agent. The agents cannot change the environment actively - in the case of Chapter 4.1 this is enforced at compile time by simply excluding it from the data an agent can emit. Note the agents change the environment implicitly by changing their state but there is no notion of an active environment process.

2. *Passive read/write* - implemented in Chapter 4.3. The environment is just shared data, which can be accessed and manipulated by the agents. Note that this forces some arbitration mechanism to prevent conflicting updates e.g. running the agents sequentially one after the other, to ensure that only one agent has access at a time.

3. *Active read/write* - as implemented above. To make it active a pure function is used where the environment data is owned by the simulation kernel and then made available to the agents through a State Monad. Another approach would be to implement the environment process as an agent, which is run together with all the other agents. This allows the environment to send and receive messages but the guarantees about when the environment will be run is lost if agents are run random sequentially.

4. *Active read-only* - can be implemented as above but instead of providing the environment data through a State Monad, a Reader Monad is used. The environment data is owned by the Simulation kernel and the process runs as a pure function as before but the data is provided in a read-only way through the Reader Monad.

5.1.3 The simulation kernel

The simulation kernel is the heart of the simulation mechanism: it holds the full simulation state and iterates the simulation step-by-step through virtual time. The full simulation state is comprised of the following:

- A mapping of agent MSFs to their id.
- A list of the current observable state of each agent.
- The state of the environment.
- A random-number generator.
- A step counter.

In each step the simulation state is used to compute the next step of the simulation and is thus updated after a state has been computed. Using pure functional programming, where we have persistent data-structures and immutable data, we can easily keep record of the simulation state for each step for debugging purposes e.g. instead of overwriting the state after each step, we can keep the state of each step and can go backwards and forwards in the time-series of steps.

The very heart of the simulation kernel is the step function, which computes the next step of the simulation. It is a *pure* function, taking the current simulation state and returns a new simulation state together with the output of the new step. The output of a step is the current simulation time, the number of events processed, the environment state and a list of the observable states of all agents.

```
type SimStepOut = (Time, Int, SugEnvironment, [AgentObservable SugAgentObservable])
-- Need RandomGen g because holding a random-number generator in SimulationState
simulationStep :: RandomGen g => SimulationState g -> (SimulationState g, SimStepOut)
```

The working horse behind *simulationStep* is another *pure* function which processes all events scheduled in the current step. It takes the list of events to process and the simulation state and returns the simulation state.

```
type EventList  = [(AgentId, ABSEvent SugEvent)]  -- from, to, event
processEvents :: RandomGen g => EventList -> SimulationState g -> SimulationState g
```

To void getting too technical and mixed up in implementation details, we provide the internals of *processEvents* in terms of steps done instead of code. The function does the following:

1. Extract the event at the front of the *EventList*. In case the list is empty, return the simulation state.
2. Look up the receivers' agent MSF in the agent mapping of the simulation state.

3. If the receiver was not found, the function ignores this and processes the next event through a recursive call.
4. If the receiver is found: run the agents' MSF and get the result.
5. Update the agents' current MSF in the mapping (note that an MSF produces a new MSF as a result!).
6. Update the agents' current observable state.
7. Handle the agents' output: create new agents and remove the agent from the simulation if it killed itself.
8. Prepend the events the agent has emitted through its output to the front *EventList* and do a recursive call to *processEvents*.

The initial *EventList* passed to *processEvents* is a list with *Tick* events scheduled for every agent, in random order. It is very important to understand that the events an agent emits, are prepended to the front of the *EventList*. This ensures that those events are processed next, which is of utmost importance for a correct working of the synchronous agent-interactions. This also implies that *processEvents* is a potentially non-terminating function, in case there is at least one agent which produces at least one event for every event it receives.

Finally we have a look at how to actually run an agents' MSF using the function *runAgentSF*. It is a *pure* function as well and thus takes all input as explicit arguments. It might look like an overkill to pass in 5 arguments and get a 6-tuple as result but this is the price we have to pay for pure functional programming: everything is explicit, with all its benefits and drawbacks.

```
runAgentSF :: RandomGen g          -- ^ RandomGen typeclass, g is a random-number generator
           => SugAgentMSF g        -- ^ The agents MSF to run.
           -> ABSEvent SugEvent    -- ^ The event it receives.
           -> ABSState             -- ^ The ABSState (next agent id and current time)
           -> SugEnvironment       -- ^ The environment state
           -> g                    -- ^ The random-number generator
           -> (SugAgentOut g, SugAgentObservable, SugAgentMSF g, ABSState, SugEnvironment, g)
runAgentSF msf evt absState env g = (ao, obs, msf', absState', env', g')
  where
    -- extract the monadic function to run
    msfAbsState = unMSF msf evt
    -- peel away one State layer: ABSState
    msfEnvState = runStateT msfAbsState absState
    -- peel away the second State layer: SugEnvironment
    msfRand     = runStateT msfEnvState env
    -- peel away the 3rd and last layer: Rand Monad
    (((((ao, obs), msf'), absState'), env'), g') = runRand msfRand g
```

Note that we run only the 3 *global* monadic layers in here, the 3 *local* layers are indeed completely local to the agent itself as shown above.

5.2 Event-Driven SIR

This short section shows how to implement the SIR model, as introduced in Chapter 2.2.1, with an event-driven approach. This is in stark contrast to the time-driven implementation in Chapter 4.1. The solutions are quantitatively equal as they produce the same class of dynamics. Qualitatively they fundamentally differ though in terms of expressivity and performance as we will see below.

To keep this section simple, we reduce code-examples as far as possible and focus on the most fundamental differences to the approach used in Sugarscape. An agent in the event-driven SIR has no output (that is: the return-type of the MSF is the empty tuple ()), because the SIR model is much less dynamic than the Sugarscape one: agents don't spawn other agents and agents can't die. Further there is no environment (see Chapter 4.1 how to add an environment to the SIR model) and observable dynamics happen not through agent-output but through side-effects.

The very heart of this implementation is the simulation state, which holds (amongst others) a priority queue and a tuple with the number of susceptible, infected and recovered agents. Agents schedule events with a time-stamp and receiver agent id, using this priority queue, which the simulation kernel processes then in order of the time-stamps to run the next agent. This is conceptionally very close to the Sugarscape implementation but events have now an additional time-stamp, which indicates the time when they are about to be scheduled - the priority queue is sorted according to the time-stamps and the simulation kernel simply processes them in order. When agents change their state they also increment / decrement the number of susceptible / infected / recovered agents, depending on which transition they make.

This makes the structure of the whole implementation much smaller than the one of Sugarscape: there is no local monad transformer stack to the agent, only a global one, which holds the simulation state as described above and the random-number monad. To get a feeling on the different approach between the Sugarscape and the SIR we show the initial function of the SIR agent. It is called by the simulation kernel to schedule initial events, adjust the simulation state and get the agents MSF.

```
-- | A sir agent is in one of three states
sirAgent :: RandomGen g
         => SIRState    -- ^ the initial state of the agent
         -> SIRAgent g  -- ^ the continuation
sirAgent Susceptible aid = do
    modifyDomainState incSus -- increment number of susceptible agents
    scheduleEvent aid MakeContact makeContactInterval -- schedule make contact event to self
    return (susceptibleAgent aid) -- return susceptible MSF
sirAgent Infected aid = do
    modifyDomainState incInf -- increment number of infected agents
    dt <- lift (randomExpM (1 / illnessDuration)) -- draw random illness duration
    scheduleEvent aid Recover dt -- schedule recovery to self
    return (infectedAgent aid) -- returns infected MSF
sirAgent Recovered _ = do
```

```
modifyDomainState incRec -- increment number of recovered agents
return recoveredAgent -- return recovered MSF
```

In the next sections we have a quick look at how we translate the time-driven susceptible, infected and recovered behaviours of into event-driven behaviours.

5.2.1 Susceptible Agent

We use the same switch mechanism of making the transition from a susceptible to an infected agent in case of an infection but how a susceptible agent gets infected works now different:

- A susceptible agent initially schedules a *MakeContact* event with $\Delta t = 1$ to itself.
- When receiving *MakeContact*, the agent sends a *Contact* event to 5 random other agents with $\Delta t = 0$. This will result in these events to be scheduled immediately. Further the agent schedules *MakeContact* with $\Delta t = 1$ to itself.
- When the agent receives a *Contact* event, it checks if it is from an infected agent. If the event is not from an infected agent, it ignores it. Otherwise it becomes infected with a given probability. In case of infection the agent decrements the number of susceptible and increments the number of infected agents.

5.2.2 Infected Agent

We use the same switch mechanism of making the transition from an infected to a recovered agent after the illness duration. The main difference is that agents send *Contact* events to each other to indicate that contacts have happened. Thus susceptible and infected agents need to react to incoming *Contact* events.

- An infected agent initially schedules a *Recover* event with a random Δt (following exponential distribution) to itself.
- When the agent receives a *Contact* event, it checks if it is from a susceptible agent. If the event is not from a susceptible agent, it ignores it. Otherwise it simply replies to this susceptible agent with a *Contact* event with $\Delta t = 0$.

5.2.3 Recovered Agent

The recovered agent does not change any more, reacts to no incoming events and schedules no events - it stays constant forever and thus outputs the empty tuple forever.

5.2.4 Reflections

Transforming a time-driven into an event-driven approach should always be possible because the ability to schedule events with time-stamps allows to map all features of time-driven ABS to an event-driven one - the discussion above should give a good direction of how this process works. Still for some models one can argue that the time-driven approach is much more expressive than an event-driven one, and we think this is certainly the case for the SIR model. The event-driven approach leads to much more fragmented logical flow and agent behaviour.

The event-driven implementation from this Chapter is around 60 - 70% faster than the time-driven implementation from Chapter 4.1, which is non-monadic and uses the FRP library Yampa. For the monadic time-driven approach of Chapter 4.3 the difference is much more dramatic: it is about 700 - 800% slower. These results dramatically highlight the problem of time-driven ABS: its performance cannot compete with an even-driven approach. This is exaggerated even more so when making use of MSFs as in Chapter 4.3. In this case, a time-driven approach becomes extremely expensive in terms of performance and one should consider an event-driven approach. In case the model is specified in a time-driven way, a transformation into an event-driven approach should always be possible as outlined above.

5.3 Discussion

This section takes a step back and reflects on various points worth noting in the event-driven approach.

5.3.1 A similar approach

After having finished our implementation, we realised that the work of [22] aimed to solve a similar problem which we also had to in this approach. The authors also use Haskell to implement ABS and more specifically looked into the use of messages and the problem of when to advance time in models with arbitrary number synchronised agent-interactions. The biggest difference is, that we approach our agents fundamentally different through the use of Monads and FRP. First in our approach an agent is only a single MSF and thus can not be directly queried for its internal state / its id or outgoing messages, instead of taking a list of messages, our agents take a single event/message and can produce an arbitrary number of outgoing messages together with an observable state - note that this would allow to query the agent for its id and its state as well by simply sending a corresponding message to the agents MSF and requiring the agent to implement message handling for it. Also the state of our agents is *completely* localised and there is no means of accessing the state from outside the agent, they are thus "fully encapsulated agents" [22]. Note that the authors of [22] define their agents with a polymorphic agent-state type s, which

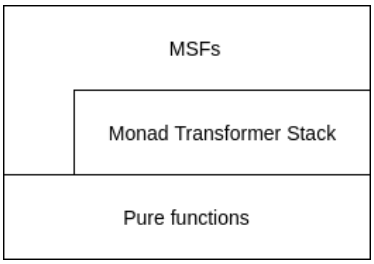


Figure 5.2: The architecture as a 3-layered system.

implies that without knowledge of the specific type of s there would be no way of accessing the state, rendering it in fact also fully encapsulated. The problem of advancing time in our approach is conceptually very similar though: after sending a tick message to each agent (in random order), we process all agents until they are idle: there are no more enqueued messages / events in the queue. The similarities in both approaches might hint at that this seems to be indeed the "right" way to go.

5.3.2 Layered architecture

The approach is designed as a 3-layered architecture, see Figure 5.2:

1. *Pure functions* are the working horses, which do the actual computations of the simulation. They are mostly used to build up the 2nd layer. Also layer 1 might access them to achieve pure computations when there is no need for effects.

2. *Monad transformer stack* (global and local) does the dirty work of effectful computation: sending messages, mutating the environment, reading model configuration, drawing random numbers, mutating agent state. This layer uses the pure functions to build up its functionality and also propagates between the 1st and 3rd layer.

3. *MSFs* (arrowized FRP) are the backbones of the architecture and define the dynamical structure of the system. This layer builds heavily on the 2nd layer and can also be seen as a highly delegation mechanism. Note that MSFs blur the distinctions between the monadic and the arrowized layer.

Separating those 3 concerns from each other makes the code more robust, easier to refactor and maintain. Further it makes code *much* easier to test as will be shown in Chapter IV.

5.3.3 Imperative nature

Both event-driven use-cases (Sugarscape and SIR) makes heavy use of the State Monad, thus one might ask what the benefits are of our pure functional ap-

proach - after all we seem to fall back into stateful, imperative style programming. On the other hand even our stateful programming is highly restricted to very specific types and operations. Further, in our monad stack we control the operations possible to the respective layers: e.g. sending messages/events is a write-only operation (as it should be), accessing the unique agent-id and the model-configuration is read-only (as it should be). All this is guaranteed at compile-time, which makes it much more manageable, maintainable, robust, composable and testable. To quote John Carmack [2]: *"A large fraction of the flaws in software development are due to programmers not fully understanding all the possible states their code may execute in."*. We claim that despite using an imperative style, the static guarantees of the types we operate on and the operations provided, it makes it easier to fully understand the possible states of the simulation code.

5.3.4 Multiple types of agents

In the Sugarscape example we have only considered one type of agents, thus the whole population is a homogeneous one in regards of the *type* of the agent. It is quite straightforward to have heterogeneous agent types as well, which is accomplished through adding additional data-declarations to the observable output and the agent-state. A consequence is that all agent types have to speak the same event-language because in regards of types the agents are treated the same way - this is also true for the monadic / effect stack: different agent types cannot have different effect types in this approach as they are seen as the same on the type level.

5.3.5 Performance

We compared an event-driven SIR implementation we did in Java to the Haskell one here. We run for 150 time-steps with 1,000 susceptible and 1 infected agent, $\beta = 5$, $\gamma = 0.05$, $\delta = 15$. Further, we fixed the random-number generators to guarantee identical dynamics in every run and averaged 8 runs. The Java implementation averages at 1.2 seconds, whereas the Haskell implementation at 6.8 seconds. These performance figures are closer than the ones in the time-driven approach of the previous chapter. This shows that event-driven is indeed much better performing and also more flexible as [108] has pointed out. Interestingly, the time-driven Java implementation outperforms the event-driven one. Although, we have improved the performance substantially compared to the time-driven approach, we address it more in-depth in the chapters on parallelism 7 and concurrency 8.

[2] `http://www.gamasutra.com/view/news/169296/Indepth_Functional_programming_in_C.php`

5.3.6 Conclusion

Overall we think that this event-driven approach is quite feasible and is *the way to go* to implement ABS in a pure functional way. The time-driven approach is quite expressive but is not as flexible and general as the event-driven one. Also performance is considerably better in event-driven approach as shown in the short section 5.2 on the event-driven SIR.

We conclude that synchronous agent-interaction was the most difficult part to figure out and get right and thus posed the greatest challenge. This concept is indeed cumbersome and clearly more complex than direct method invocation in OOP, which does the same. Unfortunately, with the goal of staying pure we do not have much other options. Note, that we didn't aim to encapsulate its complexity behind domain-specific combinators but this is certainly possible and should reduce the difficulty and complexity considerably. This is left as further research and open work which should be untertaken in the future, when putting all the concepts of this thesis into a general purpose library for pure functional ABS in Haskell.

Chapter 6

The structure of ABS computation

TODO UNFINISHED MANDATORY CHAPTER

The purpose of abstraction is not to be vague, but to create a new semantic level in which one can be absolutely precise. - Dijkstra, EWD340

generalising the structure of agent computation - with our case studies we explore them in a more practical / applied way and in this chapter we extract and distil the general concepts and abstractions behind agent computation: how can ABS, which is pure computation, can be seen structurally? This gives the ABS field for the first time a deeper understanding of the deeper structure of the computations behind agent-based simulation, which has so far always been more ad-hoc without a proper, more rigorous formulation.

pure functional computation with effects can be seen as computations over some data-structure where the data-structure defines the structure of the computation as well e.g. monoids, applicatives, monads, traversable, foldable

Note that agent-based simulation is almost always entirely pure computation without the need for direct, synchronous user-interaction or impure IO. When IO is really needed we can keep purity by creating IO actions and pass them to the simulation kernel which executes them and communicates the result back if needed - in this case only the simulation kernel needs to run in IO monad but not the agents and the environment computations.

agentout as monoid with writer: solves the Problem of iteratively constructing it the output during an event.

BUT: isnt our approach similar to the early days IO of Haskell with continuations? if this is the case we should be able to get the direct method style by writing an agent monad?

NOTE: "And a closure is just a primitive form of object: the special case of an object with just one method." https://www.tedinski.com/2018/11/20/message-oriented-programming.html

- this is still research which needs to be done by reading the papers below and

reflecting and understanding on co-monads and my implementations in general.

- can we derive an agent-monad?

https://www.javiercasas.com/articles/codata-in-action/

- what about comonads? read essence dataflow paper [154]: monads not capable of stream-based programming and arrows too general therefor comonads, we are using msfs for abs therefore streambased so maybe applicable to our approach/agents=comonads. comonads structure notions of context-dependent computation or streams, which ABS can be seen as of. this paper says that monads are not capable of doing stream functions, maybe this is the reason why i fail in my attempt of defining an ABS in idris because i always tried to implement a monad family. stopped at comonad section, continue from there. understand comonads: https://www.schoolofhaskell.com/user/edwardk/cellular-automata and https://kukuruku.co/post/cellular-automata-using-comonads/ and https://chshersh.github.io/posts/2019-03-25-comonadic-builders

- Conal Elliott has examined a comonadic formulation of functional reactive programming http://conal.net/blog/posts/functional-interactive-behavior

- comonads https://fmapfixreturn.wordpress.com/2008/07/09/comonads-in-everyday-life/

- comonads are objects very important and closely related http://www.haskellforall.com/2013/02/you-could-have-invented-comonads.html

- if conal elliott can make a comonadic formulatin of FRP and comonads are objects, then i guess i am very close to a pure functional representation of objects? pure functional objects?

independent of time-driven or event-driven, our agents are MSFs.

in fact i am deriving pure functional objects

- i have the feeling that co-algebras might be an underlying structure, which in CS come up in infinite streams - ABS can be seen as this where the agents are such streams with their output and potentially running for an infinite time, depending on the model. Ionescus thesis might reveal more information / might be an additional source on that.

In general it is easy to see why agents can not be represented by pure functions: they change over time. This is precisely what pure functions cannot do: they can't rely on some surrounding context / or on history - everything what they do is determined by their input arguments and their output. In general we have two ways of approaching this: we either have the agents changing data and behaviour internalised as we did in the previous chapters or we externalise it e.g. in the simulation kernel and provide all necessary information through arguments which was the case in the sugarscape environment.

- FREE MONADS

6.1 A Functional View

Due to the fundamentally different approaches of FP, an ABS needs to be implemented fundamentally differently, compared to established OOP approaches. We face the following challenges:

1. How can we represent an Agent, its local state and its interface?
2. How can we implement direct agent-to-agent interactions?
3. How can we implement an environment and agent-to-environment interactions?

6.1.1 Agent representation

The fundamental building blocks to solve these problems are *recursion* and *continuations*. In recursion a function is defined in terms of itself: in the process of computing the output it *might* call itself with changed input data. Continuations are functions which allow to encapsulate the execution state of a program by capturing local variables (known as closure) and pick up computation from that point later on by returning a new function. As an illustratory example, we implement a continuation in Haskell which sums up integers and stores the sum locally as well as returning it as return value for the current step:

```haskell
-- define the type of the continuation: it takes an arbitrary type a
-- and returns a type a with a new continuation
newtype Cont a = Cont (a -> (a, Cont a))

-- an instance of a continuation with type a fixed to Int
-- takes an initial value x and sums up the values passed to it
-- note that it returns adder with the new sum recursively as
-- the new continuation
adder :: Int -> Cont Int
adder x = Cont (\x' -> (x + x', adder (x + x')))

-- this function runs the given continuation for a given number of steps
-- and always passes 1 as input and prints the continuations output
runCont :: Int -> Cont Int -> IO ()
runCont 0 _ = return () -- finished
runCont n (Cont cont) = do -- pattern match to extract the function
  -- run the continuation with 1 as input, cont' is the new continuation
  let (x, cont') = cont 1
  print x
  -- recursive call, run next step
  runCont (n-1) cont'

-- main entry point of a Haskell program
-- run the continuation adder with initial value of 0 for 100 steps
main :: IO ()
main = runCont 100 (adder 0)
```

We implement an agent as a continuation: this lets us encapsulate arbitrary complex agent-state which is only visible and accessible from within the continuation - the agent has exclusive access to it. Further, with a continuation it becomes possible to switch behaviour dynamically e.g. switching from one mode of behaviour to another like in a state-machine, simply by returning new functions which encapsulate the new behaviour. If no change in behaviour should occur, the continuation simply recursively returns itself with the new state captured as seen in the example above.

The fact that we design an agent as a function, raises the question of the interface of it: what are the inputs and the output? Note that the type of the function has to stay the same (type a in the example above) although we might switch into different continuations - our interface needs to capture all possible cases of behaviour. The way we define the interface is strongly determined by the direct agent-agent interaction. In case of Sugarscape, agents need to be able to conduct two types of direct agent-agent interaction: 1. one-directional, where agent A sends a message to agent B without requiring agent B to synchronously reply to that message e.g. repaying a loan or inheriting money to children; 2. bi-directional, where two agents negotiate over multiple steps e.g. accepting a trade, mating or lending. Thus it seems reasonable to define as input type an enumeration (algebraic data-type in Haskell, see example below) which defines all possible incoming messages the agent can handle. The agents continuation is then called every time the agent receives a message and can process it, update its local state and might change its behaviour.

As output we define a data-structure which allows the agent to communicate to the simulation kernel 1. whether it wants to be removed from the system, 2. a list of new agents it wants to spawn, 3. a list of messages the agent wants to send to other agents. Further because the agents data is completely local, it also returns a data-structure which holds all *observable* information the agent wants to share with the outside world. Together with the continuation this guarantees that the agent is in full control over its local state, no one can mutate or access from outside. This also implies that information can only get out of the agent by actually running its continuation. It also means that the output type of the function has to cover all possible input cases - it cannot change or depend on the input.

```
type AgentId    = Int
data Message    = Tick Int | MatingRequest AgentGender ...
data AgentState = AgentState { agentAge :: Int, ... }
data Observable = Observable { agentAgeObs :: Int, ... }
data AgentOut   = AgentOut
  { kill       :: Bool
  , observable :: Observable
  , messages   :: [(AgentId, Message)] -- list of messages with receiver
  }
-- agent continuation has different types for input and output
newtype AgentCont inp out = AgentCont (in -> (out, AgentCont inp out))
-- taking the initial AgentState as input and returns the continuation
sugarscapeAgent :: AgentState -> AgentCont (AgentId, Message) AgentOut
sugarscapeAgent asInit = AgentCont (\ (sender, msg) ->
  case msg of
    agentCont (sender, Tick t) = ... handle tick
    agentCont (sender, MatingRequest otherGender) = ... handle mating request)
```

6.1.2 Stepping the simulation

The simulation kernel keeps track of the existing agents and the message-queue and processes the queue one element at a time. The new messages of an agent are inserted *at the front* of the queue, ensuring that synchronous bi-directional

messages are possible without violating resources constraints. The Sugarscape model specifies that in each tick all agents run in random order, thus to start the agent-behaviour in a new time-step, the core inserts a *Tick* message to each agent in random order which then results in them being executed and emitting new messages. The current time-step has finished when all messages in the queue have been processed. See algorithm **??** for the pseudo-code for the simulation stepping.

6.1.3 Environment and agent-environment interaction

The agents in the Sugarscape are located in a discrete 2d environment where they move around and harvest resources, which means the need to read and write data of environment. This is conveniently implemented by adding a State side-effect type to the agent continuation function. Further we also add a Random effect type because dynamics in most ABS in general and Sugarscapes in particular are driven by random number streams, so our agent needs to have access to one as well. All of this low level continuation plumbing exists already as a high quality library called Dunai, based on research on Functional Reactive Programming [77] and Monadic Stream Functions [122, 121].

Part III:

Parallel computation

In the introduction in Chapter 1, this thesis hypothesised that FP should allow to easily apply parallel computation to ABS - this part tries to answer this hypothesis. Thus in this part of the thesis we perform a deeper investigation on the potential of parallel programming offered by pure functional programming to apply to ABS. Another motivation this part is the notorious performance and efficiency problems of our sequential implementations (see Chapter 12.3.1), thus the work in this part can be seen as an attempt to at least mitigate the notorious performance problems of FP.

Pure functional programming as in Haskell is well known and accepted as a remedy against the difficulties and problems of parallel computation [78]. The reason for it is clear: immutable data and explicit control of side-effects removes a large class of bugs due to data-conflicts, data-races. A fundamental benefit and strength of Haskell is, that it clearly distinguishes between parallelism and concurrency *in its types* [91]. It is very important for us to do so as well:

- **Parallelism** - In parallelism, code runs in parallel solely for the purpose of doing more work within the same time, without interfering with other code through shared data (references, mutexes, semaphores,...). An example is the function *map :: (a → b) → [a] → [b]*, which maps each element of type *a* to *b* using the function *(a → b)*. It is a pure function and thus no sharing of data either through some monadic context or through the function *(a → b)* is possible. This allows to run it in parallel: each function evaluation *(a → b)* could potentially be executed at the same time, if we had enough CPU cures. Whether it runs actually in parallel or not, has no influence on the outcome, it is not subject to any non-deterministic influences. Thus we identify parallelism with pure and deterministic execution of data-transformations in parallel (data-parallelism).

- **Concurrency** - Concurrency refers to the decomposability property of a program, algorithm, or problem into order-independent or partially-ordered components or units [98]. Those parts *can* be run in parallel which as a consequence *might* give rise to asynchronous, non-deterministic events [1].

[1] Note that the functional *concurrent* programming language Erlang [6], which uses the actor model for its concurrency model, was single-threaded from its conception in 1986 until around 2008. This might sound surprising but underlines the fact that concurrency per se has nothing to do with parallel execution.

> An example are two threads, running in parallel, which share data through a reference. Depending on the scheduling and the code which is run in each thread, this gives rise to very different access patterns - the events - to the shared data, with the potential for race conditions and dirty reads. In concurrency per definition, ordering is important and the challenge of implementing parallel, concurrent programs, is to write the program in a way that despite of these non-deterministic events it is still a correctly working program. Thus we identify concurrency with parallel, impure, non-deterministic execution of imperative-style and ordered monadic evaluation.

In the next two chapters we investigate the application of both parallelism and concurrency to our pure functional ABS approach. In general, we want to see if and how parallel and concurrent programming in Haskell is transferable to pure functional ABS and what the benefits are. In particular we are interested in speeding up the existing implementations by generally developing techniques that allow us to *run agents in parallel* [2].

Note that the focus here is primarily on the conceptual nature of how to apply parallelism and concurrency to pure functional ABS, thus we refrain from doing in-depth performance analysis up-front as it is beyond the scope of this work. Still, we are very well aware that mindlessly trying to apply parallel computation can actually result in loss of performance as a problem can only be sped up in so far as we can partition it and run those partitions in parallel. Further, parallel computation comes with an overhead and if the partitioning is too fine-grained, this overhead might eat up the speed up or make it even worse. Thus, in real-world problems, performance measurements have to come first, then one can investigate where and why the performance is lost. Only if this is properly understood one can decide whether parallelism or concurrency is applicable - or none at all because the problem is actually completely sequential. As D. Knuth famously put it: *"Premature optimisation is the root of all evil"*, thus, when we see adding parallel computation as one way of optimising a problem, we need hard facts instead of wild guesses.

Besides performance improvement, we are generally interested in the implications of the way Haskell deals with parallelism and concurrency in its types. In particular we ask about the ability of keeping deterministic guarantees about the reproducibility of our simulations. We hypothesize that parallelism will allow us to retain *all* static guarantees about reproducibility *and* gives us a noticeable speed up. Further we hypothesize, that in concurrency we might see a bigger speed up but sacrifice the very guarantee about reproducibility. However, we assume that by using Haskell's unique approach to Software Transactional Memory (STM), we don't lose this guarantee completely - it will just get weakened by guaranteeing that the non-deterministic influence is through concurrency only *and nothing else*.

[2] Note that we use the term *parallel* to identify both *parallelism* and *concurrency* and we distinguish between them whenever necessary using their respective terms.

Chapter 7

Parallelism in ABS

The promise of parallelism in Haskell is compelling: speeding up the execution but retaining all static compile-time guarantees about determinism. In other words, using parallelism could give us a substantial performance improvement without sacrificing the static guarantees of reproducible outputs from repeated runs with initial conditions.

Generally, parallelism can be applied whenever the execution of code is order-independent, that is referential transparent, and has no implicit or explicit side-effects. In this section we introduce the two most important parallelism concepts of Haskell, *evaluation* and *data-flow* parallelism, and discuss their potential use in pure functional ABS in general. We follow [105] and refer to it for an in-depth discussion. Further, we show how these concepts can be added to our previously discussed use-cases of Chapters 4.1, 4.3 and Sugarscape 5.1 and compare their performance over the original sequential approaches.

7.1 Evaluation Parallelism

Evaluation parallelism introduces so called strategies to evaluate lazy data-structures in parallel. Examples are strategies to evaluate a list, or tuples in parallel where for each element a spark is created. The fundamental concept Haskell uses to achieve evaluation parallelism is its own non-strictness nature. Non-strictness means that expressions are not eagerly evaluated when defined, like in imperative programming languages but only evaluated when their result is actually needed. This is implemented internally using thunks, which are pointers to expressions. When the value of an expression is needed, this thunk is accessed and the expression is reduced until the next constructor or lambda is encountered. This is called Weak Head Normal Form (WHNF) evaluation because it only reduces the "head" of the expression, which could consist of sub expressions. This indirection, the separation of data creation from consumption / evaluation, indeed enables evaluation parallelism and Haskell provides two additional functions to support this:

- *par* :: $a \to b \to b$ Returns the second argument b but evaluates the first argument a in parallel. It is used when the result of evaluating a is required later.
- *seq* :: $a \to b \to b$ - Returns the second argument b but is strict in its first argument, which means it forces its evaluation to WHNF. It is used when the result of evaluating a is required now.

Internally, evaluation parallelism is handled through so called *sparks*, which are basically thunks which get evaluated in parallel. The Haskell runtime system manages sparks and distributes them to threads where they get executed. Due to their extremely light-weight nature, it is no problem to create tens of thousands of sparks. One has to bear in mind that even though evaluating in parallel through sparks is extremely cheap, it still has some overhead. Thus, the workload of each element in a list might be too low for a spark, then one can distribute chunks of a list onto a single spark. It is important to understand, that all this works without side-effects - the strategy combinators are all pure functions building on *par* and *seq*. This allows us to add parallelism to an algorithm by applying a parallel evaluation strategy to its result which e.g. is a lazy list - again this is possible through non-strictness, which separates the construction of data from its consumption.

7.1.1 Evaluation Parallelism In ABS

Using compositional parallelism is exactly what we use to aim at adding evaluation parallelism for agent execution in the non-monadic SIR example 4.1. We know that the whole simulation is a completely pure computation because Yampa is non-monadic, thus it is guaranteed that there are no side-effects - thus agents are run conceptually in parallel e.g. using map. Now we should be able to add parallelism without needing to re-implement *dpSwitch* which is the function which runs the agents in parallel (Also re-implementing switch functions would not get us very far because of WHNF evaluation it is the wrong end to start parallel evaluation: probably only the arguments would be evaluated but not the agent behaviour.)

The solution is to add evaluation parallelism in the agent-output collection phase: where the recursive switch into the *stepSimulation* function happens. There we use a evaluation strategy to evaluate the outputs of all agents in parallel. The agents will then be evaluated in parallel due to compositional parallelism, when we force the output of each in parallel. We give more details in the short case-study 7.3.1 below.

7.2 Data-flow parallelism

When relying on a lazy data structure to apply parallelism is not an option, evaluation strategies as presented before are not applicable. Further, although lazy evaluation brings compositional parallelism, it makes it hard to reason

about performance. Data-flow parallelism offers an alternative over evaluation strategies, where the programmer can give more details but gains more control: data dependencies are made explicit and reliance on lazy evaluation is avoided [106]. Data-flow parallelism is implemented through the *Par* Monad, which provides combinators for expressing data-flows: in this monad it is possible to *fork* parallel tasks which communicate with each other through shared locations, so called *IVar*s. Internally these tasks are scheduled by a work-stealing scheduler which distributes the work evenly on available processors at runtime. *IVars* behave like futures or promises: they are initially empty and can be written once. Reading from an empty *IVar* will cause the calling task (or main thread) to wait until it is filled. An example is a parallel evaluation of two fibonacci numbers:

```
runPar (do
  i <- new             -- create new IVar
  j <- new             -- create new IVar
  fork (put i (fib n)) -- fork new task compute fib n and put result into IVar i
  fork (put j (fib m)) -- fork new task compute fib m and put result into IVar j
  a <- get i           -- wait for the result from IVar i and collect it
  b <- get j           -- wait for the result from IVar j and collect it
  return (a,b)         -- return the sum
```

Note that with this it is also possible to express parallel evaluation of a list or a tuple as with evaluation strategies. The difference though is, that it does avoid lazy evaluation. More importantly, putting a value into an *IVar* requires the type of the value to have an instance of the *NFData* typeclass. This simply means that a value of this type can be fully evaluated, not just to WHNF but to evaluate the full expression the value represents.

7.2.1 Data-flow parallelism in ABS

The Par monad seems to be a very suitable mechanism to enable agents to express data-flow parallelism within their behaviour. This is only possible with the monadic ABS approach as in the SIR implementation of Chapter 4.3 and the Sugarscape of Chapter 5.1. An important fact is that if the Par monad is used, it has to be the innermost monad because it cannot be a transformer. This is emphasised by the fact that there exists no ParT transformer instance, like for other monads (e.g. StateT, RandT, ReaderT,... we used in the Sugarscape chapter). Making the Par monad a transformer would have (probably) the meaning of running the *bind* in parallel. It is quite clear that this simply makes no sense: *bind* is a function for composing / sequencing monadic actions, which in general involves side-effects of some kind. Side-effects inherently impose some sequencing where evaluation of different sequences has different meanings in general - thus the sequential nature of *bind*. Thus follows that running monadic code in parallel is simply not possible in general due to side-effects [1] and thus there is no (meaningful) way to put the Par into a transformer stack.

[1] Besides, it would be not very clear what we are running in parallel within the *bind* operator as there is nothing to parallelise in general e.g. no structure over which we can parallelise in general.

7.3 Case-Studies

In this section we go a little bit more into detail how we applied the parallelism concepts as already outline above to our use-cases from Chapters 4.1, 4.3 and Sugarscape 5.1. We only show briefly the technical details and refer to the full code in footnotes. Note that all timings are rough averages over multiple runs and not precise measurements because that is not the point here. We are only interested in showing what rough potential there is for speeding up computation through deterministic parallelism - we are not interested in high performance computation here but rather in conceptual comparisons between sequential and parallel implementations.

7.3.1 Non-Monadic SIR

Evaluation Strategies As outlined above we want to apply parallelism to agent evaluation by composing the output with parallel evaluation by slightly changing the function *switchingEvt*. This function receives the output of all agents from the current simulation step and generates an event to recursively switch back into *stepSimulation* to compute the next simulation step. The code is as follows:

```
switchingEvt :: SF ((), [SIRState]) (Event [SIRState])
switchingEvt = arr (\ (_, newAs) -> parEvalAgents newAs)
  where
    -- NOTE: need a seq here otherwise would lead to GC'd sparks because
    -- the main thread consumes the output already when aggregating, so using seq
    -- will force parallel evaluation at that point
    parEvalAgents :: [SIRState] -> Event [SIRState]
    parEvalAgents newAs = newAs' `seq` Event newAs'
      where
        -- NOTE: chunks of 200 agents seem to deliver the best performance
        -- when we are purely CPU bound and don't have any IO
        newAs' = withStrategy (parListChunk 200 rseq) newAs
        -- NOTE: alternative is to run every agent in parallel
        -- only use when IO of simulation output is required
        -- newAs' = withStrategy (parList rseq) newAs
```

Which evaluation strategy resulted in the best performance increase turned out to depend on how we observe the results of the simulation. Due to Haskells non-strict nature, as long as no output is *observed*, nothing would get computed ever. We have developed three (3) different ways to observe the output of this simulation and thus we measured the timings for all of them:

1. Printing the output of the last simulation step. This requires to run the simulation for the whole 150 time-steps because each step depends on the output of the previous one. Because the simulation is completely CPU bound, the best performance increase turned out to run agents in batches where for this model 200 seems to deliver the best performance. If each agent is run in parallel, we still achieved a substantial performance increase but not as high as the batched version. An analysis showed that around

Output type	Parallel	Sequential	Factor
Print of last step (1)	3.9	16.38	4.24
Writing simulation output (2)	9.41	10.17	1.08
Appending current step (3)	9.73	10.04	1.03
(1) and (2) combined	5.02	19.68	3.92

Table 7.1: Timings of parallel vs. sequential non-monadic SIR.

1.5 million (!) sparks got created but most of them were never evaluated. There is a limit in the spark pool and we have obviously hit that.

2. Writing the aggregated output of the whole simulation to an export file. This requires in principle to run the simulation through but due to non-strictness, the writing to the export file begins straight away. This interferes with parallelism due to system calls which get interleaved with parallelism, leading to less performance increase than the previous one. It turned out that in this case running each agent in parallel didn't lead to reduced performance, because we are IO bound (see below).

3. Appending the aggregated output of the current step to an export file. This is necessary when we have a very long running simulation for which we want to write each step out (more or less) as soon as it is computed. The function which runs this simulation is tail-recursive and can thus run forever, which is not possible in the previous case where the function is not necessarily tail-recursive and aggregates the outputs. Here we use a strategy which evaluates each agent in parallel as well.

4. A combined approach of 1 and 2 where the output of the last simulation step is printed and then the aggregate is written to a file.

The timings are reported in Table 7.1. All timings were measured with 1000 agents running for 150 time-steps, and $\Delta = 0.1$. We performed 8 runs and report the timings in seconds. The parallel version was compiled with the '-threaded' option and used all 8 cores with the '-N' option. For the sequential implementation the '-threaded' option was removed as well as the evaluation strategies - it is purely sequential code. All experiments were carried out on the same machine [2]

The table clearly indicates, that in case we are purely CPU bound we get a quite impressive speed up of 4.24 on 8 cores - parallelism clearly pays off here, especially after it is so easy to add. On the other hand it seems that as soon as we are IO bound, the parallelism performance benefit is completely wasted. This does not come as a surprise and it is well established that generally as soon as IO is involved, performance benefits from parallelism will suffer. This point will be addressed by the use of concurrency where due to concurrent evaluation

[2]Dell XPS 13 (9370) with Intel Core i7-8550U (8 cores), 16 GB Ram (plugged in).

the IO is decoupled from the computation, making the latter one completely CPU bound and resulting in an impressive speed-up in such a case as well.

What comes a bit as a surprise is that in the case of the sequential implementation, the CPU bound implementation, which does no IO is actually slower than the ones which do IO. This can be attributed to lazy evaluation which seems to increase performance because IO can be performed actually while the simulation computes the next step, interleaving the evaluation and IO. Thus when comparing the parallel CPU bound approach (1) to the IO bound sequential ones (2) and (3) results in a lower speed up factor of roughly 2.6. The combined approach (4) then shows that we actually can have the substantial speed up of CPU bound (1) but still write the result to the file like in (2). This is of fundamental importance in simulation, because after all they often produce massive amounts of data which need to be stored somewhere.

Par Monad The book [105] mentions that Par Monad and evaluation strategies result roughly in the same performance in most of the benchmarks. And indeed: we also applied Par Monad here to run the agents in parallel by evaluating their output and we get about the same speed up in cases (1) and (4). The IO bound cases (2) and (3) perform slower: (2) is nearly 50% slower than its evaluation strategy pendant and (3) is about 25% slower. What is interesting is, that running all agents in their own task seems to be fine here in any case whereas it was slower in the evaluation strategy in the CPU bound case:

```
-- NOTE: with the Par monad, splitting the list into chunks seems not
-- to be necessary - we get the same speed up as in evaluation strategies
parMonadAgents :: [SIRState] -> Event [SIRState]
parMonadAgents newAs = Event (runPar (do
  -- simply return the value of the agent, resulting in a deepseq due to
  -- NFData instance of put in IVar
  ivs <- mapM (spawn . return) newAs
  mapM get ivs))
```

7.3.2 Monadic SIR

We can try to apply the same techniques of parallelising the agents as we did in the previous section in the non-monadic version of the SIR model. There is but a fundamental problem in this case, as we have already outlined in the section on data-flow parallelism: we are running the simulation in the monadic context of a ReaderT and Random Monad stack. In monadic execution, depending on the monad (stack), we deal with side-effects, which immediately necessitates the ordering of execution: whether an effectful expression is evaluated before another one can have indeed very fundamental differences and in general we have to assume that it does. Indeed: the way the agents are evaluated is through the *mapM* function, which evaluates them sequentially applying their side-effects in sequence. It does not matter that the agents behave as if they are run in parallel without the possibility to interfere with each other, the simple fact that they are run within the ReaderT(Rand g) transformer stack requires sequencing. It is not the ReaderT which causes the delicate issue, it is rather the Rand

monad, which basically behaves like a State monad with the random-number generator as internal state, which gets updated with each draw. Due to this sequential evaluation, we can hypothesize that our approach is doomed from the beginning and that we will not see any speed up when we apply parallelism - on the contrary, we can expect the performance to be worse with it due to the overhead caused by it.

Indeed, when we put our hypotheses to a test [3] we see exactly that behaviour: the sequential implementation, which does not use any parallelism and is not compiled with the -threaded option takes on average 41.76 seconds to finish. When adding parallelism with evaluation strategies in the same way as we did in non-monadic SIR, we end up with 49.63 seconds on average to finish - a clear performance *decrease*! For the Par monad approach its even worse, which averages at 52.98 seconds to finish. These timings clearly show that 1) agents which are run in a monadic context with *mapM* are not applicable to parallelism, 2) the parallelism mechanisms add a substantial overhead which is in accordance with the reports in [105].

Still we don't give up completely and want to see if running the agents sequentially but some Par monadic code *within* them could gain us some speed up. The function we target is the neighbourhood querying function, which looks up the 8 (moore) surrounding neighbours of an agent. It is a pure function and uses *map* and is thus perfectly suitable to parallelism. We simply extend the transformer stack by putting the Par monad innermost and then run the *neighbours* function within the Par monad:

```
-- type simplified for explanatory reasons
neighbours :: Disc2dCoord -> SIREnv -> Par [SIRState]
neighbours (x, y) e = do
    ivs <- mapM (\c -> spawn (return (e ! c))) nCoords
    mapM get ivs
  where
    nCoords = ... -- create neighbours coordinates
```

Unfortunately the performance is even worse than without it, averaging at 66.68 seconds to finish. The workload seems to be too low for parallelism to pay off. Further, when keeping the Par monad as innermost monad but using the original pure *neighbours* function without Par we arrive at an average of 55.9 seconds to finish when running multi threaded on 8 cores and 45.56 seconds when compiled with threading enabled but running on a single core. These measurements demonstrate that using the Par monad and parallelism in general can lead to an impressively *reduced* performance, compared to a sequential implementation, due do massive overhead and too fine-grained parallelism.

This leaves us basically without any options of parallelism for the monadic SIR model, we will come back to this use-case in the concurrency section, where we will show that by using concurrency it is possible to achieve a substantial speed up by orders of magnitude.

[3] We used the same experiment setup as in the non-monadic implementation.

7.3.3 Sugarscape

As already shown in the case of the monadic SIR implementation from the previous section, running agents in parallel within a monadic context does not bring us any speed up - on the contrary, we get penalised with a substantial performance loss due to the overhead incurred by adding parallelism. Further, running the agents in the Par monad alone incurs also a substantial overhead, thus ultimately these roads are dead ends for our Sugarscape implementation as well.

This leaves us only with a very minor thing we could optimize in the Sugarscape model: the behaviour of the environment, which is a pure computation, using maps and folds [4] over an *IntMap*. It might look like we are out of luck as it seem that we cannot parallelise the updating of an IntMap but the work of [105] shows that it is indeed possible through a combination of the Par monad and the *Applicative* typeclass. The *IntMap* provides the function *traverseWithKey :: Applicative t ⇒ (Key → a → t b) → IntMap a → t (IntMap b)*. We can use this whenever we need to traverse the whole IntMap to update every cell in the list. The obvious use-case for this is the regrowing of resources (sugar and spice) in every step. Unfortunately, this parallelism makes the performance worse than the sequential - obviously the regrowing of resources is not computation heavy and the parallelism incurs more overhead than the speed up it provides.

Another thing we can parallelise is the computation of the pollution diffusion which uses a standard map to compute the new pollution level of each cell. Using *'withStrategy (parList rseq)'* is applied to the list of all cells but the parallelism is too fine-grained: we actually get worse performance than without it - another case for premature optimisation without hard facts profiling.

Thus we end up with the same conclusion as with the monadic SIR implementations: there is practically no opportunity to parallelise the implementation and we refer to the concurrency chapter where we show how to achieve performance improvements in orders of magnitude when we employ concurrency instead of parallelism.

7.4 Parallel Runs

Often one needs to perform a large number of runs of the same simulation. The most prominent use-cases for this are:

- Parameter Sweeps / Variations - To explore the parameter space and the dynamics under varying parameter configurations, the same simulation is run with varying parameters and the results recorded for statistical analysis.

[4] In general, folds can be parallelized only when the operation being folded is associative, and then the linear fold can be turned into a tree. Although applicable, we don't follow that approach here and leave it for further research.

- Stochastic replications - Due to ABS stochastic nature, running a simulation only once does not allow to generalise or predict overall behaviour - one might have just hit an (un)fortunate special case. To counter this problem, in ABS multiple replications of the simulation are run with same initial model parameters but with different random-number streams. All the results are collected and analysed stochastically (averaged, median,...) from which then more general properties can be derived.

In each case thousands of runs of the same simulation with different model parameters and / or varying random-number streams are needed, requiring a considerable amount of computing power.

Parallelism is a remedy to this problem because in each of these cases individual runs do not interfere with each other and thus can be seen as isolated from each other, like referential, pure computations. Our approaches shown in the Part II make this very explicit: the top level functions can always be made pure computations because we are ruling out IO (so far) and thus even though Monads are employed in many cases, they are still pure. A benefit of our approach is that it is guaranteed at compile time, that individual runs do not interfere with each other and thus there is no danger that parallel runs influence each other.

All this allows to implement parameter sweeps and stochastic replications both through evaluation and data-flow parallelism making another very compelling use-case - probably the most striking one - for the use of parallelism in ABS. We hypothesize that data-flow parallelism is better suited for this task because it makes parallelism more explicit as it is indeed a data-flow problem: we pass parameters to single replications which are run and return their results. To apply this we simply run the top level replication logic in the Par Monad where replications are run in parallel by forking tasks and results are handed back through IVars. If we want the convenience of having a monadic random-number generator within the Par monad as well, one can use the combined ParRand monad which provides both.

7.5 Discussion

In this chapter we briefly explored how to apply parallelism to our pure functional ABS approach and ran case studies on our existing models to get a rough estimate of what performance increase we can expect. In general, we aimed at running agents in parallel, employing both techniques of evaluation and data-flow parallelism. Because of the quite sequential nature of the agent behaviour itself, there is much less potential for parallelism *within* an agent, thus the idea was to run them all in parallel. This should create enough workload as an agent is an obvious unit of partitioning which can indeed be run in parallel under given circumstances.

Although we showed how to apply the techniques, unfortunately the case studies showed that performance improvement was only possible in the case of

the non-monadic SIR as introduced in Chapter 4.1. The speed up stemmed from the fact that the agents ran indeed in parallel as our original goal was, thus resulting in a significant speed up factor of over 4.

Unfortunately all attempts in parallelising the monadic SIR and Sugarscape implementations failed, which was expected. As soon as we switch to monadic agents, evaluation parallelism is out of the window, as agents can't be run in parallel any more because side-effects require to impose a sequential ordering (which is exactly what the meaning of a Monad is).

We further showed how to apply parallelism *within* an SIR agent and for updating the environment of the Sugarscape in parallel using the *Par* monad. It didn't show any speed up as well but this was not the primary objective: we rather explored conceptually to demonstrate how it can be used - other models might benefit massively from such an approach as they might contain much more potential for data-flow parallelism.

We didn't discuss data parallelism on large array structure or parallelism on GPU as they are used in massively large numerical computation. These techniques achieve tremendous speed ups but are not applicable to ABS in general but only in very model specific cases where e.g. each agent needs to crunch through arrays of numbers to perform numerical computations. We refer to [105] for a more in-depth discussion of both in Haskell and leave the application to pure functional ABS for further research.

Concluding, we see a direct consequence of the fact that types reflect the semantics of our model: when our agents are pure they can be run in parallel and independent from each other but if they are monadic, then they are not applicable to parallelism. In the next chapter, we show how to approach this problem and come up with a solution where we can run monadic agents in parallel. This is the only possible within a concurrent context, which means we have to sacrifice determinism in our solution. Still, by favouring Software Transactional Memory using the STM monad instead of resorting to IO we get the guarantee that the the only source of non-determinism is due to the concurrency of STM *and nothing else*. Further, we will show that an additional benefit of using STM over IO is that the STM approach reaches a considerable higher speed up compared to a lock-based approach based on IO.

Chapter 8

Concurrent ABS

In an ideal world, we would like to solve all our problems using parallelism but unfortunately, it can't be applied to all parallel problems and ABS is no exception. As soon as there are data-dependencies, like we have them in the Sugarscape model in the form of the read/write environment and synchronous agent-interactions, and to a lesser extent in the monadic SIR with the Rand monad, we cannot avoid concurrency. More general, this is due to the fact that agents are executed within a monadic context, from which the sequencing of effectful computations immediately follows - the very meaning of the Monad abstraction. Indeed, we have shown both by argument and measurement in the previous chapter the very fact that parallelism is simply not applicable to monadic execution of agents due to sequencing of effects, which renders all attempts of running monadic agents in parallel void. In this chapter we discuss the use of concurrency to run agents which have a monadic context in parallel - which is the only way we can execute monadic agents at the same time.

Traditional approaches to concurrency follow a lock-based approach, where sections which access shared data are synchronised through synchronisation primitives like mutexes, semaphores, monitors,... The lock-based path is a well trodden one, with all problems and benefits well established. In this chapter we follow a different path and look into using Software Transactional Memory (STM) for implementing concurrent ABS, which promises to overcome the problems of lock-based approaches. Although STM exists in other languages as well, Haskell was one of the first to natively build it into its core, thus it is a natural choice to follow that direction when already investigating pure functional ABS.

Unfortunately, as soon as we employ concurrency, we lose all static guarantees about reproducibility and the use of STM is no exception. Still, STM has the unique benefit that it can guarantee the lack of persistent side-effects at compile time, allowing unproblematic retries of transactions, something of fundamental importance in STM as will be described below. This implies also another *very* compelling advantage of STM over unrestricted lock-based approaches: by using STM, we can reduce the side-effects allowed substantially

and guarantee at compile time, that the differences between runs of same initial conditions will only stem from the fact that we run the simulation concurrently - *and from nothing else*. All this makes the use of STM very compelling and to our best knowledge we are the very first to investigate the use of STM for implementing concurrent ABS in a systematic way.

The paper [45] gives a good indication how difficult and complex constructing a correct concurrent program is and shows how much easier, concise and less error-prone an STM implementation is over traditional locking with mutexes and semaphores. More important, it shows that STM consistently outperforms the lock-based implementations. We follow this work and compare the performance of lock-based and STM implementations and hypothesise that the reduced complexity and increased performance will be directly applicable to ABS as well.

We present two case studies using the already introduced SIR (Chapter 2.2.1) and Sugarscape (Chapter 2.2.2) models. We compare the performance of lock-based and STM implementations in each case where we investigate both the scaling performance under increasing number of CPUs and agents. We show that the STM implementations consistently outperform the lock-based ones and scale much better to increasing number of CPUs both on local machines and on Amazon Cloud Services.

8.1 Software Transactional Memory

Software Transactional Memory (STM) was introduced by [137] in 1995 as an alternative to lock-based synchronisation in concurrent programming which, in general, is notoriously difficult to get right. This is because reasoning about the interactions of multiple concurrently running threads and low level operational details of synchronisation primitives is *very hard*. The main problems are:

- Race conditions due to forgotten locks;
- Deadlocks resulting from inconsistent lock ordering;
- Corruption caused by uncaught exceptions;
- Lost wake-ups induced by omitted notifications.

Worse, concurrency does not compose. It is very difficult to write two functions (or methods in an object) acting on concurrent data which can be composed into a larger concurrent behaviour. The reason for it is that one has to know about internal details of locking, which breaks encapsulation and makes composition dependent on knowledge about their implementation. Therefore, it is impossible to compose two functions e.g. where one withdraws some amount of money from an account and the other deposits this amount of money into a different account: one ends up with a temporary state where the money is in

none of either accounts, creating an inconsistency - a potential source for errors because threads can be rescheduled at any time.

STM promises to solve all these problems for a low cost by executing actions *atomically*, where modifications made in such an action are invisible to other threads and changes by other threads are invisible as well until actions are committed - STM actions are atomic and isolated. When an STM action exits, either one of two outcomes happen: if no other thread has modified the same data as the thread running the STM action, then the modifications performed by the action will be committed and become visible to the other threads. If other threads have modified the data then the modifications will be discarded, the action block rolled-back and automatically restarted.

8.1.1 STM in Haskell

The work of [70, 71] added STM to Haskell, which was one of the first programming languages to incorporate STM into its main core and added the ability to composable operations. There exist various implementations of STM in other languages as well (Python, Java, C#, C/C++, etc) but we argue, that it is in Haskell with its type-system and the way how side-effects are treated where it truly shines.

In the Haskell implementation, STM actions run within the *STM* context. This restricts the operations to only STM primitives as shown below, which allows to enforce that STM actions are always repeatable without persistent side-effects because such persistent side-effects (e.g. writing to a file, launching a missile) are not possible in an *STM* context. This is also the fundamental difference to *IO*, where all bets are off because *everything* is possible as there are basically no restrictions because *IO* can run everything.

Thus the ability to *restart* a block of actions without any visible effects is only possible due to the nature of Haskells type-system: by restricting the effects to STM only, ensures that no uncontrolled effects, which cannot be rolled-back, occur.

STM comes with a number of primitives to share transactional data. Amongst others the most important ones are:

- *TVar* - A transactional variable which can be read and written arbitrarily;
- *TMVar* - A transactional *synchronising* variable which is either empty or full. To read from an empty or write to a full *TMVar* will cause the current thread to block and retry its transaction when *any* transactional primitive of this block has changed.
- *TArray* - A transactional array where each cell is an individual transactional variable *TVar*, allowing much finer-grained transactions instead of e.g. having the whole array in a *TVar*;
- *TChan* - A transactional channel, representing an unbounded FIFO channel, based on a linked list of *TVar*.

Further STM also provides combinators to deal with blocking and composition:

- *retry :: STM ()* - Retries an *STM* block. This will cause to abort the current transaction and block the thread it is running in. When *any* of the transactional data primitives has changed, the block will be run again. This is useful to await the arrival of data in a *TVar* or put more concretely, to block on arbitrary conditions.
- *orElse :: STM a → STM a → STM a* - Allows to combine two blocking operations where either one is executed but not both. The first operation is run and if it is successful its result is returned. If it retries, then the second is run and if that one is successful its result is returned. If the second one retries, the whole orElse retries. This can be used to implement alternatives in blocking conditions, which can be obviously nested arbitrarily.

To run an *STM* action the function *atomically :: STM a → IO a* is provided, which performs a series of *STM* actions atomically within an *IO* context. It takes the STM action which returns a value of type *a* and returns an *IO* action which returns a value of type *a*. This *IO* action can only be executed within an *IO* context, either within the main-thread or an explicitly forked thread.

STM in Haskell is implemented using optimistic synchronisation, which means that instead of locking access to shared data, each thread keeps a transaction log for each read and write to shared data it makes. When the transaction exits, the thread checks whether it has a consistent view to the shared data or not: whether other threads have written to memory it has read.

In the paper [72] the authors use a model of STM to simulate optimistic and pessimistic STM behaviour under various scenarios using the AnyLogic simulation package. They conclude that optimistic STM may lead to 25% less retries of transactions. The authors of [124] analyse several Haskell STM programs with respect to their transactional behaviour. They identified the roll-back rate as one of the key metric which determines the scalability of an application. Although STM might promise better performance, they also warn of the overhead it introduces which could be quite substantial in particular for programs which do not perform much work inside transactions as their commit overhead appears to be high.

8.1.2 An example

We provide a short example to demonstrate the use of STM. To make it more interesting and to show the retry semantics, we use it within a *StateT* transformer where *STM* is the innermost monad. It is important to understand that STM does not provide a transformer instance for very good reasons. If it would provide a transformer then we could make *IO* the innermost monad and perform IO actions within STM. This would violate the retry semantics as in case of a retry, STM is unable to undo the effects of IO actions in general. This stems

from the fact, that the IO type is simply too powerful and we cannot distinguish between different kinds of IO actions in the type, be it simply reading from a file or actually launching a missile. Lets look at the example code:

```
stmAction :: TVar Int -> StateT Int STM Int
stmAction = do
  -- print a debug output and increment the value in StateT
  Debug.trace "increment!" (modify (+1))
  -- read from the TVar
  n <- lift (readTVar v)
  -- await a condition: content of the TVar >= 42
  if n < 42
    -- condition not met: retry
    then lift retry
    -- condition met: return content ot TVar
    else return n
```

In this example, the *STM* is the innermost monad in a stack with a *StateT* transformer. When the *stmAction* is run, it prints an "increment!" debug message to the console and increments the value in the *StateT* transformer. Then it awaits a condition: as long as *TVar* is less then 42 the action will retry whenever it is run. If the condition is met, it will return the content of the *TVar*. We see the combined effects of using the transformer stack: we have both the *StateT* and the *STM* effects available. The question is how this code behaves if we actually run it. To do this we need to spawn a thread:

```
stmThread :: TVar Int -> IO ()
stmThread v = do
  -- the initial state of the StateT transformer
  let s = 0
  -- run the state transformer with initial value of s (0)
  let ret = runStateT stmAction s
  -- atomically run the STM block
  (a, s') <- atomically ret

  putStr ("final StateT state     = " ++ show s')
  putStrLn (", STM computation result = " ++ show a)
```

The thread simply runs the *StateT* transformer layer with the initial value of 0 and then the STM computation through *atomically* and prints the result to the console. Note that *a* is the result of *stmAction* and *s'* is the final state of the *StateT* computation. To actually run this example we need the main-thread to updated the *TVar* until the condition is met within *stmAction*:

```
main :: IO ()
main = do
  -- create a new TVar with initial value of 0
  v <- newTVarIO 0
  -- start the stmThread and pass the TVar
  forkIO (stmThread v)

  forM_ [1..42] (\i -> do
    -- use delay to 'make sure' that a retry is happening for ever increment
    threadDelay 10000
```

```
-- write new value to TVar using atomically
atomically (writeTVar v i))
```

If we run this program, we will see "increment!" printed 43 times, followed by "final StateT state = 1, STM computation result = 42". This clearly demonstrates the retry semantics: *stmAction* is retried 42 times and thus prints "increment" 43 times to the console. The *StateT* computation however is carried out only once and is always rolled back when a retry is happening. The rollback is easily possible in pure functional programming due to persistent data-structure: simply throw away the new value and retry with the original value. This example also demonstrates that any IO actions which happen within an STM block are persistent and can obviously not be rolled back - Debug.trace is an IO action masked as pure using *unsafePerformIO*.

8.2 STM in ABS

In this section we give a short overview of how we apply STM in our ABS. In both case-studies we fundamentally follow a time-driven, parallel approach as introduced in Chapter 3.2, where the simulation is advanced by a given Δt and in each step all agents are executed. To employ parallelism, each agent runs within its own thread and agents are executed in lock-step, synchronising between each Δt, which is controlled by the main thread. See Figure 8.1 for a visualisation of our concurrent, time-driven lock-step approach.

By running each agent in a thread will guarantee the execution in parallel even if the agent has a monadic context. This is forces us to evaluate each agents monadic context separately instead of running them all in a common context. Note that ultimately we are ending up in the *IO* context because *STM* can be only transacted from within an *IO* context due to non-deterministic side-effects. This is no contradiction to our original claim: yes we are running in IO but not the agent behaviour itself, which is a fundamental difference.

An agent thread will block until the main-thread sends the next Δt and runs the *STM* action atomically with the given Δt. When the *STM* action has been committed, the thread will send the output of the agent action to the main-thread to signal it has finished. The main thread awaits the results of all agents to collect them for output of the current step e.g. visualisation or writing to a file.

As will be described in subsequent sections, central to both case-studies is an environment which is shared between the agents using a *TVar* or *TArray* primitive through which the agents communicate concurrently with each other. To get the environment in each step for visualisation purposes, the main thread can access the *TVar* and *TArray* as well.

8.2.1 Adding STM to agents

We briefly discuss how to add STM to agents on a technical level and also show how to run them within their own threads. We use the SIR implementation as

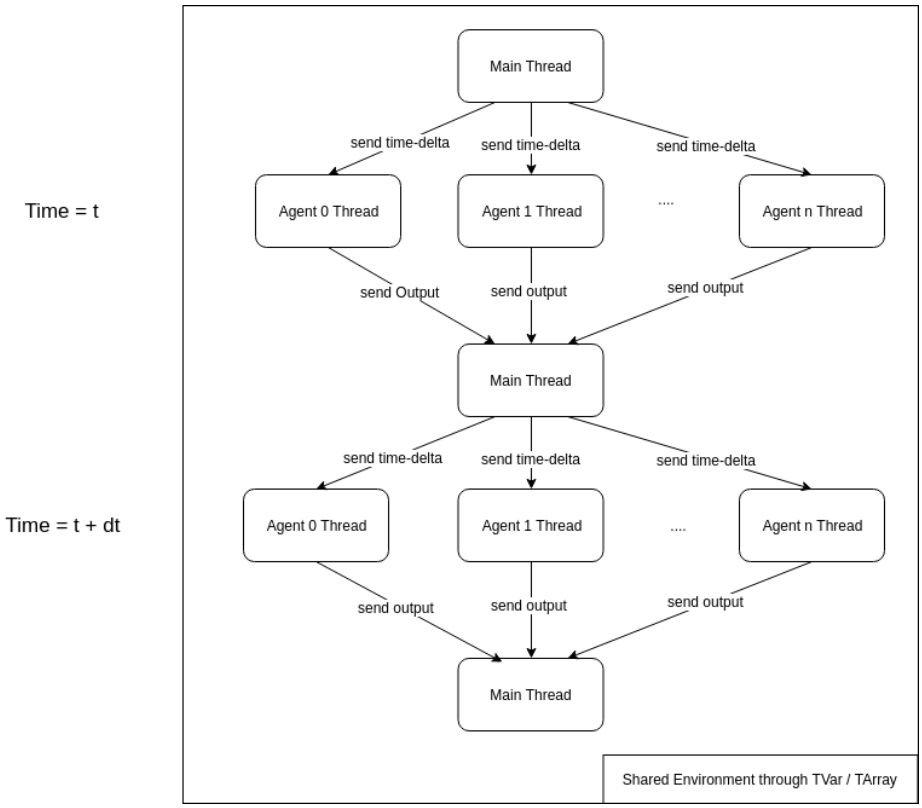


Figure 8.1: Diagram of the parallel time-driven lock-step approach.

example - applying it to the Sugarscape implementation works exactly the same way and is left as a trivial exercise to the reader.

The first step is to simply add the *STM* monad on the *innermost* level to already the existing transformer stack. Further, the environment is now passed as a transactional data primitive to the agent at *construction time*. Thus the agent does not receive the *SIREnv* as input any more but receives it through currying when constructing its initial Signal Function. Further, the agent modifies the *SIREnv* directly through the *TVar*, as demonstrated in the case of the infected agent.

```
-- Make Rand a transformer to be able to add STM as innermost monad
type SIRMonad g = RandT g STM
-- Input to agent is now an empty tuple instead of the Environment
type SIRAgent g = SF (SIRMonad g) () SIRState

-- The signal function construction function takes now the TVar
-- with the environment.
sirAgent :: RandomGen g => TVar SIREnv -> Disc2dCoord -> SIRState -> SIRAgent g

-- The infected agent behaviour is nearly the same except that
-- the agent modifies the environment through the TVar
infected :: RandomGen g => SF (SIRMonad g) () (SIRState, Event ())
infected = proc _ -> do
  recovered <- occasionally illnessDuration () -< ()
  if isEvent recovered
    then (do
              -- updated the environment through the TVar
      arrM_ (lift $ lift $ modifyTVar env (changeCell coord Recovered)) -< ()
      returnA -< (Recovered, Event ()))
    else returnA -< (Infected, NoEvent)
```

The agent thread is straight forward: it takes *MVar* synchronisation primitives to synchronise with the main-thread and simply runs the agent behaviour each time it receives the next *DTime*:

```
agentThread :: RandomGen g
            => Int              -- ^ Number of steps to compute
            -> SIRAgent g       -- ^ Agent behaviour signal function
            -> g                -- ^ Random-number of the agent
            -> MVar SIRState    -- ^ Synchronisation back to main-thread
            -> MVar DTime       -- ^ Receiving DTime for next step
            -> IO ()
agentThread 0 _ _ _ _ = return () -- all steps computed, terminate thread
agentThread n sf rng retVar dtVar = do
  -- wait for dt to compute current step
  dt <- takeMVar dtVar

  -- compute output of current step
  let sfReader = unMSF sf ()
      sfRand   = runReaderT sfReader dt
      sfSTM    = runRandT sfRand rng
  -- run the STM action atomically within IO
  ((ret, sf'), rng') <- atomically sfSTM

  -- post result to main thread
```

```
  putMVar retVar ret

  -- to next step
  agentThread (n - 1) sf' rng retVar dtVar
```

Computing a simulation step is now trivial within the main-thread: all agent threads *MVar*s are signalled to unblock followed by an immediate block on the *MVar*s into which the agent threads post back their result. The state of the current step is then extracted from the environment, which is stored within the *TVar* which the agent threads have updated.

```
simulationStep :: TVar SIREnv
               -> [MVar DTime]
               -> [MVar SIRState]
               -> DTime
               -> IO SIREnv
simulationStep env dtVars retVars dt = do
  -- tell all threads to continue with the corresponding DTime
  mapM_ (`putMVar` dt) dtVars
  -- wait for results but ignore them, SIREnv contains all states
  mapM_ takeMVar retVars
  -- return state of environment when step has finished
  readTVarIO env
```

The difference to an implementation which uses IO are minor but far reaching. Instead of using *STM* as innermost monad, we use *IO*, thus running the whole agent behaviour within the IO monad. Instead of receiving the environment through a *TVar*, the agent receives it through an *IORef*. It also receives an *MVar* which is the synchronisation primitive to synchronise the access to the environment in the *IORef* amongst all agents. Agents grab and release the synchronisation lock of the *MVar* when they enter and leave a critical section in which they operate on the environment stored in the *IORef*.

8.3 Case Study I: SIR

Our first case study is the SIR model as introduced in Chapter 2.2.1. The aim of this case study is to investigate the potential speed up a concurrent *STM* implementation gains over a sequential one under varying number of CPU cores and agents. The behaviour of the agents is quite simple and the interactions are happening indirectly through the environment, where reads from the environment outnumber the writes to it by far. Further, a comparison to a lock-based implementation with the *IO* monad is done to understand that *STM* is also able to outperform traditional concurrency, *in a pure functional ABS setting* while still retaining its greater static guarantees than *IO* [1].

1. Sequential - This is the original implementation as discussed in Chapter 4.3 where the discrete 2D grid is shared amongst all agents as read-only

[1] The code of all three implementations is available at `https://github.com/thalerjonathan/phd/tree/master/public/stmabs/code/SIR`

OS	Fedora 28, 64-bit
RAM	16 GByte
CPU	Intel i5-4670K @ 3.4GHz
HD	250Gbyte SSD
Haskell	GHC 8.2.2

Table 8.1: Machine and Software specs for all experiments

	Cores	Duration
Sequential	1	72.5
Lock-Based	1	60.6
	2	42.8
	3	38.6
	4	41.6
STM	1	53.2
	2	27.8
	3	21.8
	4	**20.8**

Table 8.2: Experiments on 51x51 (2,601 agents) grid with varying number of cores.

data and the agents are executed sequentially within the main thread without any concurrency.

2. STM - This is the same implementation as the *Sequential* one but agents run now in the *STM* monad and have access to the discrete 2D grid through a transactional variable *TVar*. This means that the agents now communicate indirectly by reads and writes through the *TVar*.

3. Lock-Based - This follows the *STM* implementation, with the agents running in *IO*. They share the discrete 2D grid using an *IORef* and have access to an *MVar* lock to synchronise access to it.

Each experiment was run until $t = 100$ and stepped using $\Delta t = 0.1$. For each experiment we conducted 8 runs on our machine (see Table 8.1) under no additional work-load and report the mean. In the experiments we varied the number of agents (grid size) as well as the number of cores when running concurrently - the numbers are always indicated clearly.

8.3.1 Constant Grid Size, Varying Cores

In this experiment we held the grid size constant to 51 x 51 (2,601 agents) and varied the cores. The results are reported in Table 8.2.

The *STM* implementation running on 4 cores shows a speed up factor of 3.6 over *Sequential*, which is a quite impressive number when considering that we

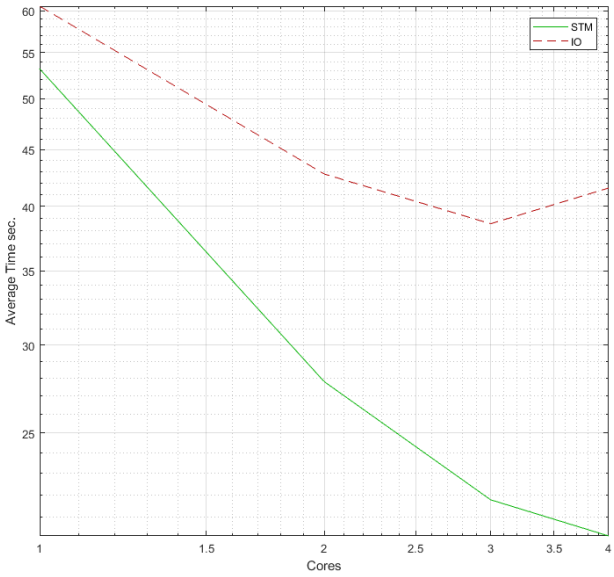


Figure 8.2: Comparison of performance and scaling on multiple cores of STM and Lock-Based. Note that the Lock-Based implementation seems to perform slightly worse on 4 than on 3 cores probably due to lock-contention.

can achieve at most a factor of 4 when running on 4 cores. It seems that *STM* allow us to push the practical limit very close to the theoretical one, whereas the *Lock-Based* approach just arrives at a factor of 1.74 on 4 cores.

Comparing the performance and scaling to multiple cores shows that the *STM* implementation significantly outperforms the *Lock-Based* one and scales better to multiple cores. The *Lock-Based* implementation performs best with 3 cores and shows slightly worse performance on 4 cores as can be s een in Figure 8.2. This is no surprise because the more cores are running at the same time, the more contention for the lock, thus the more likely synchronisation happening, resulting in higher potential for reduced performance. This is not an issue in *STM* because no locks are taken in advance.

8.3.2 Varying Grid Size, Constant Cores

In this experiment we varied the grid size and used always 4 cores. The results are reported in Table 8.3 and plotted in Figure 8.3.

It is clear that the *STM* implementation outperforms the *Lock-Based* implementation by a substantial factor.

Grid-Size	STM	Lock-Based	Ratio
51 x 51 (2,601)	**20.2**	41.9	2.1
101 x 101 (1,0201)	**74.5**	170.5	2.3
151 x 151 (22,801)	**168.5**	376.9	2.2
201 x 201 (40,401)	**302.4**	672.0	2.2
251 x 251 (63,001)	**495.7**	1,027.3	2.1

Table 8.3: Performance on varying grid sizes.

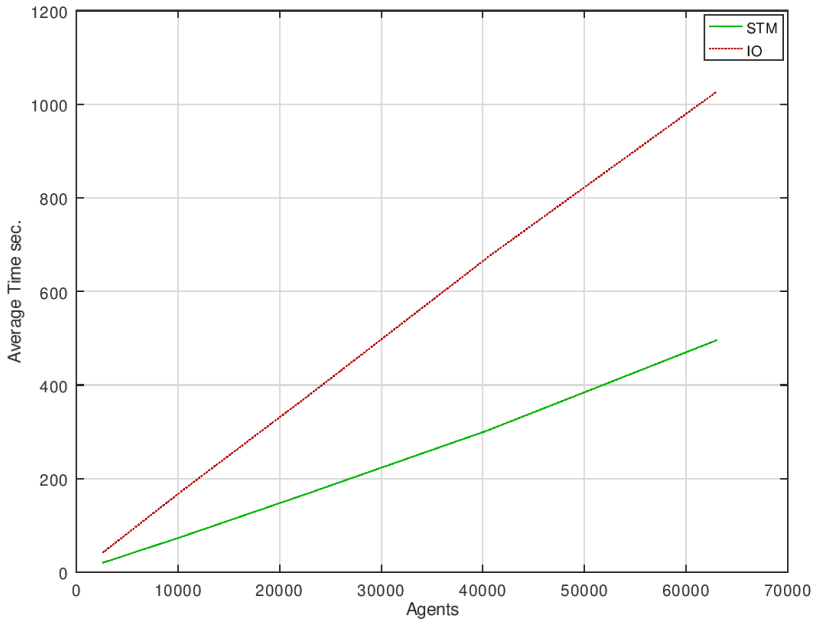


Figure 8.3: Performance on varying grid sizes.

Grid-Size	Commits	Retries	Ratio
51 x 51 (2,601)	2,601,000	1306.5	0.0
101 x 101 (10,201)	10,201,000	3712.5	0.0
151 x 151 (22,801)	22,801,000	8189.5	0.0
201 x 201 (40,401)	40,401,000	13285.0	0.0
251 x 251 (63,001)	63,001,000	21217.0	0.0

Table 8.4: Retry ratios on varying grid sizes on 4 cores.

	Cores	51x51	251x251
Lock-Based	16	72.5	1830.5
	32	73.1	1882.2
STM	16	**8.6**	**237.0**
	32	12.0	248.7

Table 8.5: Performance on varying cores on Amazon S2 Services.

8.3.3 Retries

Of very much interest when using STM is the retry-ratio, which obviously depends highly on the read-write patterns of the respective model. We used the *stm-stats* library to record statistics of commits, retries and the ratio. The results are reported in Table 8.4.

Independent of the number of agents we always have a retry-ratio of 0.0. This indicates that this model is *very* well suited to STM, which is also directly reflected in the much better performance over the *Lock-Based* implementation. Obviously this ratio stems from the fact, that in our implementation we have *very* few writes, which happen only in case when an agent changes from Susceptible to Infected or from Infected to Recovered. On the other hand, there are a very large number of reads due to indirect agent interaction. For *STM* this is no problem because no lock is taken but the *Lock-Based* approach is forced to conservatively take the lock to ensure mutual exclusive access to the critical section across all agents.

8.3.4 Going Large-Scale

To test how far we can scale up the number of cores in both the *Lock-Based* and *STM* cases, we ran two experiments, 51x51 and 251x251, on Amazon EC2 instances with a larger number of cores than our local machinery, starting with 16 and 32 to see if we are running into decreasing returns. The results are reported in Table 8.5.

As expected, the *Lock-Based* approach doesn't scale up to many cores because each additional core brings more contention to the lock, resulting in an even more decreased performance. This is particularly obvious in the 251x251 experiment because of the much larger number of concurrent agents. The *STM*

approach returns better performance on 16 cores but fails to scale further up to 32 where the performance drops below the one with 16 cores. In both STM cases we measured a retry-ratio of 0, thus we assume that with 32 cores we become limited by the overhead of STM transactions [124] because the workload of an STM action in our SIR implementation is quite small.

Compared to the *Sequential* implementation, *STM* reaches a speed up factor of 8.4 on 16 cores, which is still impressive but is much further away from the theoretical limit than in the case of only 4 cores - a further indication that this model in particular and our approach in general does not scale up arbitrarily.

8.3.5 Discussion

The timing measurements speak a clear language: running in *STM* and sharing state using a transactional variable *TVar* is much more time-efficient than both the *Sequential* and *Lock-Based* approach. On 4 cores *STM* achieves a speed up factor of 3.6, nearly reaching the theoretical limit. Obviously both *STM* and *Lock-Based* sacrifices determinism: repeated runs might not lead to same dynamics despite same initial conditions. Still, by sticking to *STM*, we get the guarantee that the source of this non-determinism is concurrency within the *STM* monad but *nothing else*. This we is something we can not guarantee in the case of the *Lock-Based* approach as all bets are off when running within *IO*. It seems that we are quite lucky to have *both* the better performance *and* the stronger static guarantees in the *STM* approach.

8.4 Case Study II: Sugarscape

The second case study is the Sugarscape model as introduced in Chapter 2.2.2. In this case study we look into the potential performance improvement in a model with much more complex agent behaviour and dramatically increased writes on the shared environment.

We implemented the *Carrying Capacity* (p. 30) section of Chapter II of the Sugarscape book [49]. In each step agents search (move) to the cell with the most sugar they see within their vision, harvest all of it from the environment and consume sugar because of their metabolism. Sugar regrows in the environment over time. Only one agent can occupy a cell at a time. Agents don't age and cannot die from age. If agents run out of sugar due to their metabolism, they die from starvation and are removed from the simulation. The authors report that the initial number of agents quickly drops and stabilises around a level depending on the model parameters. This is in accordance with our results as we show in Chapter IV and guarantees that we don't run out of agents. The model parameters are as follows:

- Sugar Endowment: each agent has an initial sugar endowment randomly uniform distributed between 5 and 25 units;

- Sugar Metabolism: each agent has a sugar metabolism randomly uniform distributed between 1 and 5;
- Agent Vision: each agent has a vision randomly uniform distributed between 1 and 6, same for each of the 4 directions (N, W, S, E);
- Sugar Growback: sugar grows back by 1.0 unit per step until the maximum capacity of a cell is reached;
- Agent Number: initially 500 agents;
- Environment Size: 50 x 50 cells with toroid boundaries which wrap around in both x and y dimension.

Note that in this implementation (as in the full Chapter II of the book), no direct and no synchronous agent-interactions as we implemented them in Chapter 5.1 are happening. As in the SIR example, all agents interact with each other indirectly through the shared environment. This allows us to regard the implementation as a time-driven, parallel one wherein each step agents act conceptually at the same time.

We compare four different implementations [2]:

1. Sequential - All agents are run after another (including the environment) and the environment is shared amongst the agents using a *StateT* transformer.
2. Lock-Based - All agents are run concurrently in the *IO* monad and the environment is shared between the agents, using an *IORef* with the access synchronised through an *MVar* lock.
3. STM TVar - All agents are run concurrently in the *STM* monad and the environment is shared using a *TVar* between the agents.
4. STM TArray - All agents are run concurrently in the *STM* monad and the environment is shared using a *TArray* between the agents.

We follow [100] and measure the average number of steps per second of the simulation over 60 seconds. For each experiment we conducted 8 runs on our machine (see Table 8.1) under no additional work-load and report the average. In the experiments we varied the number of cores when running concurrently - the numbers are always indicated clearly.

Ordering The model specification requires to shuffle agents before every step (Footnote 12 on page 26 [49]). In the *Sequential* approach we do this explicitly but in the *Lock-Based* and both *STM* approaches we assume this to happen automatically due to race-conditions in concurrency, thus we arrive at an effectively shuffled processing of agents: we implicitly assume that the order of the

[2] The code is freely available at `https://github.com/thalerjonathan/phd/tree/master/public/stmabs/code/SugarScape`

	Cores	Steps	Retries
Sequential	1	39.4	N/A
Lock-Based	1	43.0	N/A
	2	51.8	N/A
	3	57.4	N/A
	4	58.1	N/A
STM *TVar*	1	**47.3**	0.0
	2	53.5	1.1
	3	57.1	2.2
	4	53.0	3.2
STM *TArray*	1	45.4	0.0
	2	**65.3**	0.02
	3	**75.7**	0.04
	4	**84.4**	0.05

Table 8.6: Steps per second and retries on 50x50 grid with 500 initial agents on varying cores.

agents is *effectively* random in every step. The important difference between the two approaches is that in the *Sequential* approach we have full control over this randomness but in the *STM* not - also this means that repeated runs with the same initial conditions might lead to slightly different results. This decision leaves the execution order of the agents ultimately to Haskell's Runtime System and the underlying OS. We are aware that by doing this, we make assumptions that the threads run uniformly distributed (fair) but such assumptions should not be made in concurrent programming. As a result we can expect this fact to produces non-uniform distributions of agent runs but we assumed that for this model this does not has a significance influence - in case of doubt, we could resort to shuffling the agents before running them in every step. We agree that this very problem would deserve in-depth research on its own, where also the influence of non-deterministic ordering on the correctness and results of ABS has to be analysed. This is not the main interest of this section though and we leave it for further research as it is completely beyond the focus of this thesis.

8.4.1 Constant Agent Size

In a first approach we compare the performance of all implementations on varying numbers of cores. The results are reported in Table 8.6 and plotted in Figure 8.4.

As expected, the *Sequential* implementation is the slowest, followed by the *Lock-Based* and *TVar* approach whereas *TArray* is the best performing one.

We clearly see that using a *TVar* to share the environment is a very inefficient choice in this model: *every* write to a cell leads to a retry independent whether the reading agent reads that changed cell or not, because the data-structure can

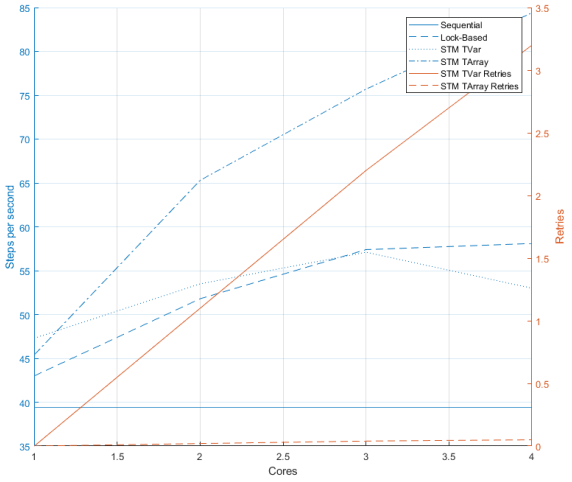


Figure 8.4: Steps per second and retries on 50x50 grid and 500 initial agents on varying cores.

not distinguish between individual cells. By using a *TArray* we can avoid the situation where a write to a cell in a far distant location of the environment will lead to a retry of an agent which never even touched that cell. Also the *TArray* seems to scale up by 10 steps per second for every core added. It will be interesting to see how far this could go with the Amazon experiment, as we seem not to hit a limit with 4 cores yet.

The inefficiency of *TVar* is also reflected in the nearly similar performance of the *Lock-Based* implementation which even outperforms it on 4 cores. This is due to very similar approaches because both operate on the whole environment instead of only the cells as *TArray* does. This seems to be a bottleneck in *TVar* reaching the best performance on 3 cores, which then drops on 4 cores due to an increasing retries ratio. The *Lock-Based* approach seems to reduce its returns on increased number of cores hitting a limit at 4 cores as well.

8.4.2 Scaling up Agents

So far we kept the initial number of agents at 500, which due to the model specification, quickly drops and stabilises around 200 due to the carrying capacity of the environment as described in the book [49] section *Carrying Capacity* (p. 30).

We now want to measure the performance of our approaches under increased number of agents. For this we slightly change the implementation: always when an agent dies it spawns a new one which is inspired by the ageing and birthing feature of Chapter III in the book [49]. This ensures that we keep

Agents	Sequential	Lock-Based	TVar (3 cores)	TVar (4 cores)	TArray
500	14.4	20.2	20.1	18.5	**71.9**
1,000	6.8	10.8	10.4	9.5	**54.8**
1,500	4.7	8.1	7.9	7.3	**44.1**
2,000	4.4	7.6	7.4	6.7	**37.0**
2,500	5.3	5.4	9.2	8.9	**33.3**

Table 8.7: Steps per second on 50x50 grid with varying number of agents with 4 (and 3) cores except Sequential (1 core).

the number of agents roughly constant (still fluctuates but doesn't drop to low levels) over the whole duration. This ensures a constant load of concurrent agents interacting with each other and demonstrates also the ability to terminate and create concurrent agents (threads) dynamically during the simulation.

Except for the *Sequential* approach we ran all experiments with 4 cores (TVar with 3 as well). We looked into the performance of 500, 1,000, 1,500, 2,000 and 2,500 (maximum possible capacity of the 50x50 environment). The results are reported in Table 8.7 and plotted in Figure 8.5.

As expected, the *TArray* implementation outperforms all others substantially. Also as expected, the *TVar* implementation on 3 cores is faster than on 4 cores as well when scaling up to more agents. The *Lock-Based* approach performs about the same as the *TVar* on 3 cores because of the very similar approaches: both access the *whole* environment. Still the *TVar* approach uses one core less to arrive at the same performance, thus strictly speaking outperforming the *Lock-Based* implementation.

What seems to be very surprising is that in the *Sequential* and *TVar* cases the performance with 2,500 agents is *better* than the one with 2,000 agents. The reason for this is that in the case of 2,500 agents, an agent can't move anywhere because all cells are already occupied. In this case the agent won't rank the cells in order of their pay-off (max sugar) to move to but just stays where it is. We hypothesize that due to Haskells laziness the agents actually never look at the content of the cells in this case but only the number which means that the cells themselves are never evaluated which further increases performance. This leads to the better performance in case of *Sequential* and *TVar* because both exploit laziness. In the case of the *Lock-Based* approach we still arrive at a lower performance because the limiting factor are the unconditional locks. In the case of the *TArray* approach we also arrive at a lower performance because it seems that STM perform reads on the neighbouring cells which are not subject to lazy evaluation. In Haskell it is notoriously difficult to reason about efficiency and this behaviour of improved performance due to Haskells lazyness is no exception. We leave an in-depth investigation for further research as it is beyond the focus of this chapter.

We also measured the average retries both for *TVar* and *TArray* under 2,500 agents where the *TArray* approach shows best scaling performance with 0.01

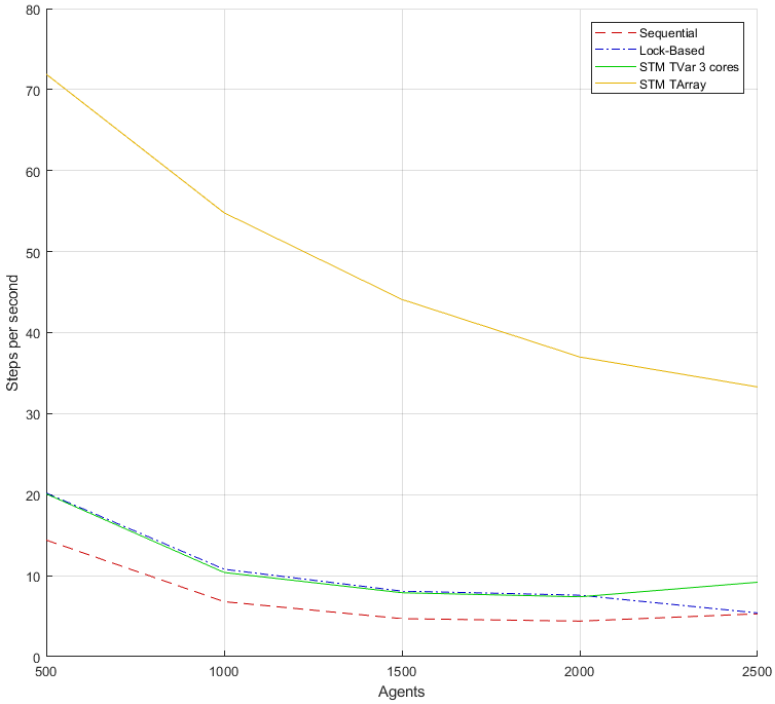


Figure 8.5: Steps per second on 50x50 grid and varying number of agents with 4 (and 3) cores except Sequential (1 core).

	Cores	Carrying Capacity	Rebirthing
Lock-Based	16	53.9	4.4
	32	44.2	3.6
STM TArray	16	**116.8** (0.23)	**39.5** (0.08)
	32	**109.8** (0.41)	**31.3** (0.18)

Table 8.8: Steps per second on varying cores on Amazon S2 Services.

retries whereas *TVar* averages at 3.28 retries. Again this can be attributed to the better transactional data-structure which reduces retry-ratio substantially to near-zero levels.

8.4.3 Going Large-Scale

To test how far we can scale up the number of cores in both the *Lock-Based* and *TArray* cases, we ran the two experiments (carrying capacity and rebirthing) on Amazon EC2 instances with increasing number of cores starting with 16 and 32 to see if we run into decreasing returns. The results are reported in Table 8.8.

As expected, the *Lock-Based* approach doesn't scale up to many cores because each additional core brings more contention to the lock, resulting in even more decreased performance. This is particularly obvious in the rebirthing experiment because of the much larger number of concurrent agents. The *TArray* approach returns better performance on 16 cores but fails to scale further up to 32 where the performance drops below the one with 16 cores. We indicated the retry-ratio in brackets and see that they roughly double from 16 to 32, which is the reason why performance drops as at this point.

8.4.4 Comparison with other approaches

The paper [100] reports a performance of 17 steps in RePast, 18 steps in MASON (both non-parallel) and 2,000 steps per second on a GPU on a 128x128 grid. Although our *Sequential* implementation, which runs non-parallel as well, outperforms the RePast and MASON implementations of [100], one must be very well aware that these results were generated in 2008, on current hardware of that time.

The very high performance on the GPU does not concern us here as it follows a very different approach than ours. We focus on speeding up implementations on the CPU as directly as possible without locking overhead. When following a GPU approach one needs to map the model to the GPU which is a delicate and non-trivial matter. With our approach we show that speed up with concurrency is very possible without the low-level locking details or the need to map to GPU. Also some features as bilateral trading between agents, where a pair of agents needs to come to a conclusion over multiple synchronous steps, is difficult to implement on a GPU whereas this is easily possible using STM.

Note that we kept the grid-size constant because we implemented the environment as a single agent which works sequentially on the cells to regrow the sugar. Obviously this doesn't really scale up on parallel hardware and experiments which we haven't included here due to lack of space, show that the performance goes down dramatically when we increase the environment to 128x128 with same number of agents which is the result of Amdahl's law where the environment becomes the limiting factor of the simulation. Depending on the underlying data-structure used for the environment we have two options to solve this problem. In the case of the *Sequential* and *TVar* implementation we build on an indexed array, which we can be updated in parallel using the existing data-parallel support in Haskell. In the case of the *TArray* approach we have no option but to run the update of every cell within its own thread. We leave both for further research as it is out of scope of this paper.

8.4.5 Discussion

This case study showed clearly that besides being substantially faster than the *Sequential* implementation, *STM* is also able to perform considerably better than a *Lock-Based* approach even in the case of a model with much higher complexity in agent behaviour and dramatically increased number of writes to the environment. Further, this case study demonstrated that the selection of the right transactional data-structure is of fundamental importance when using *STM*. Selecting the right transactional data-structure is very model-specific and can lead to dramatically different performance results. In this case the *TArray* performed best due to many writes but in the SIR case-study a *TVar* showed good enough results due to the very low number of writes. When not carefully selecting the right transactional data-structure which supports fine-grained concurrency, a lock-based implementation might perform as well or even outperform the STM approach as can be seen when using the *TVar*. Although the *TArray* is the better transactional data-structure overall, it might come with an overhead, performing worse on low number of cores than a *TVar* approach but has the benefit of quickly scaling up to multiple cores. Depending on the transactional data-structure, scaling up to multiple cores hits a limit at some point. In the case of the *TVar* the best performance is reached with 3 cores. With the *TArray* we reached this limit around 16 cores.

Note that the comparison between the *Lock-Based* approach and the *STM TArray* implementation is a bit unfair due to a very different locking structure. A more suitable comparison would have been to use an indexed Array with a tuple of (MVar, IORef) in each cell to support fine-grained locking on cell-level. This would be a more just comparison to the *STM Array* where fine-grained transactions happen on the cell-level. We hypothesize that *STM* will still outperform the *IO* approach but to a lesser degree - we leave the proof of this for further research.

8.5 Discussion

In this chapter we have shown how to apply concurrency to monadic ABS to gain substantially speed up. We developed a novel approach, using Software Transactional Memory (STM), which to our best knowledge has not been discussed systematically in the context of ABS so far. This new approach outperforms a traditional lock-based implementation running in the *IO* monad *and* guarantees that the differences between runs with same initial conditions stem from the non-determinism within *STM but nothing else*. The latter point can't be guaranteed by the lock-based approach as it runs in the *IO* monad, which allows literally anything from reading from a file, to launching a missile. Further, with SFM, concurrency becomes more a control-flow oriented concern, so using STM allows us to treat the concurrent problem within an agent as a data-flow oriented one without cluttering the model code with operational details of concurrency. This gives strong evidence that *STM* should be favoured over lock-based approaches in general for implementing concurrent ABS in Haskell.

Note that in this chapter we assumed that concurrent execution has no qualitative influence on the dynamics: although repeated runs with same initial conditions (might) lead to different results due to non-determinism, the dynamics follow still the same distribution as the one from the sequential implementation. To verify this we can make use the techniques of property-based testing as shown in Chapter 10 but we leave it for further research.

The next step would be to add synchronous agent-interactions as they occur in the Sugarscape use-cases of mating, trading and lending. We have started to do work on this already and could implement also one-directional agent-interactions as they occur in the disease transmission, payback of loans and notification of inheritance upon the death of a parent agent. We use the *TQueue* primitive to emulate the behaviour of mailboxes through which agents can post events to each other. The result is promising but needs more investigation. We have also started looking into synchronous agent-interactions using STM which is a lot trickier and is very susceptible to dead-locks (which are still possible in STM!). We have yet to prove how to implement reliable synchronous agent-interactions without deadlocks in *STM*. It might be very well the case that a truly concurrent approach is doomed due to the following [105] (Chapter 10. Software Transactional Memory, "What Can We Not Do with STM?"): *"In general, the class of operations that STM cannot express are those that involve multi-way communication between threads. The simplest example is a synchronous channel, in which both the reader and the writer must be present simultaneously for the operation to go ahead. We cannot implement this in STM, at least compositionally, for the same reason that we cannot implement TMVar with fairness: the operations need to block and have a visible effect — advertise that there is a blocked thread — simultaneously."*.

Further, *STM* is not fair because *all* threads, which block on a transactional primitive, have to be woken up, thus a FIFO guarantee cannot be given. We hypothesize that for most models, where the *STM* approach is applicable, this

has no qualitative influence on the dynamics as agents are assumed to act conceptually at the same time and no fairness is needed. We leave the test of this hypothesis for future research.

We didn't look into applying distributed computation to our approach. One direction to follow would be to use the *Cloud Haskell* library, which is very similar to the concurrency model in Erlang. We leave this for further research as it is completely beyond the scope of this thesis.

Part IV:

Property-Based testing

Introduction

When implementing an Agent-Based Simulation (ABS) it is of fundamental importance that the implementation is correct up to some specification and that this specification matches the real world in some way. This process is called verification and validation (V&V), where *validation* is the process of ensuring that a model or specification is sufficiently accurate for the purpose at hand whereas *verification* is the process of ensuring that the model design has been transformed into a computer model with sufficient accuracy [132]. In other words, validation determines if we are we building the *right model*, and verification if we are building the *model right* up to some specification [13].

One can argue that ABS should require more rigorous programming standards than other computer simulations [126]. The fact that researchers in ABS are looking for an emergent behaviour in the dynamics of the simulation, they are always tempted to look for surprising behaviour and expect something unexpected from their simulation. Also, due to ABS' *constructive / exploratory* nature [47, 48], there exists some uncertainty about the dynamics the simulation will produce before running it. The authors [117] see the current process of building ABS as a discovery process where models of an ABS often lack an analytical solution in general, which makes verification much harder if there is no such solution. Thus it is often very difficult to judge whether an unexpected outcome can be attributed to the model or has in fact its roots in a subtle programming error [58].

In general this implies that it is not possible to prove that a model is valid in general but that the best we can do is to *raise the confidence* in the correctness of the simulation. Therefore, the process of V&V is not the proof that a model is correct but it is the *process* of trying to show that the model is *not incorrect*. The more checks one carries out which show that it is not incorrect, the more confidence we can place in the models validity. To tackle such a problem in software, software engineers have developed the concept of test-driven development (TDD).

Test-Driven Development (TDD) was popularised in the early 00s by Kent Beck [15] as a way to a more agile approach to software-engineering, where instead of doing each step (requirements, implementation, testing,...) as separated from each other, all of them are combined in shorter cycles. Put shortly, in TDD tests are written for each feature before actually implementing it, then the feature is fully implemented and the tests for it should pass. This cycle is re-

peated until the implementation of all requirements has finished. Traditionally TDD relies on so called unit tests which can be understood as a piece of code which when run isolated, tests some functionality of an implementation. Thus we can say that test-driven development in general and unit testing together with code-coverage in particular, guarantee the correctness of an implementation to some informal degree, which has been proven to be sufficiently enough through years of practice in the software industry all over the world.

Related Work

The work [36] was the first to discuss how to apply TDD to ABS, using unit testing to verify the correctness of the implementation up to a certain level. They show how to implement unit tests within the RePast Framework [112] and make the important point that such a software needs to be designed to be sufficiently modular otherwise testing becomes too cumbersome and involves too many parts. The paper [7] discusses a similar approach to DES in the AnyLogic software toolkit.

The paper [116] proposes Test Driven Simulation Modelling (TDSM) which combines techniques from TDD to simulation modelling. The authors present a case study for maritime search-operations where they employ ABS. They emphasise that simulation modelling is an iterative process, where changes are made to existing parts, making a TDD approach to simulation modelling a good match. They present how to validate their model against analytical solutions from theory using unit tests by running the whole simulation within a unit test and then perform a statistical comparison against a formal specification.

The paper [67] gives an in-depth and detailed overview over verification, validation and testing of agent-based models and simulations and proposes a generic framework for it. The authors present a generic UML class model for their framework which they then implement in the two ABS frameworks RePast and MASON. Both of them are implemented in Java and the authors provide a detailed description how their generic testing framework architecture works and how it utilises unit testing with JUnit to run automated tests. To demonstrate their framework they provide also a case study of an agent-base simulation of synaptic connectivity where they provide an in-depth explanation of their levels of test together with code.

Towards Property-Based Testing

According to [44], unit testing in Haskell is quite common and robust. Although generally speaking unit tests tend to be of less importance in Haskell since the type system makes an enormous amount of invalid programs completely inexpressible by construction. Unit tests tend to be written later in the development lifecycle and generally tend to be about the core logic of the program and not the intermediate plumbing [44]. Although it would be interesting to see how we

can apply unit testing to our approach, it is straight forward, nothing new and does not constitute unique research.

Thus, in this chapter we introduce an additional technique for TDD: *property-based testing*, which can be seen complementary to unit testing. Property-based testing has its origins in Haskell [31, 32, 133], where it was first conceived and implemented. It has been successfully used for testing Haskell code for years and also been proven to be useful in the industry [83]. We show and discuss how this technique can be applied to test pure functional ABS implementations. To our best knowledge property-based testing has never been looked at in the context of ABS and this thesis is the first one to do so.

The main idea of property-based testing is to express model-specifications and laws directly in code and test them through *automated* and *randomised* test-data generation. Thus one hypothesis of this thesis is that due to ABS *stochastic* and *exploratory / generative / constructive* nature, property-based testing is a natural fit for testing ABS in general and pure functional ABS implementations in particular. It thus should pose a valuable addition to the already existing testing methods in this field, worth exploring.

To substantiate and test our hypothesis, we conducted a few case-studies. First, we look into how to express and test agent specifications for both the time- and event-driven SIR implementations in Chapter 9. Then we show how to encode model invariants of the SIR implementation and validate it against the formal specification from SD using property-tests in Chapters 10 and 11. Note that we explicitly exclude obvious applications of property-testing like boundary-checks of the environment, helper functions of agents,... as although they are used within ABS, there is nothing new in testing them.

Note that property-based testing has a close connection to model-checking [107], where properties of a system are proved in a formal way. The important difference is that the checking happens directly on code and not on the abstract, formal model, thus one can say that it combines model-checking and unit testing, embedding it directly in the software-development and TDD process without an intermediary step. We hypothesise that adding it to the already existing testing methods in the field of ABS is of substantial value as it allows to cover a much wider range of test-cases due to automatic data generation. This can be used in two ways: to verify an implementation against a formal specification and to test hypotheses about an implemented simulation. This puts property-based testing on the same level as agent- and system testing, where not technical implementation details of e.g. agents are checked like in unit tests but their individual complete behaviour and the system behaviour as a whole.

The work [116] explicitly mentions the problem of test coverage which would often require to write a large number of tests manually to cover the parameter ranges sufficiently enough - property-based testing addresses exactly this problem by *automating* the test-data generation. Note that this is closely related to data-generators [67], load generators and random testing [29]. Property-based testing though goes one step further by integrating this into a specification language directly into code, emphasising a declarative approach and pushing the

generators behind the scenes, making them transparent and focusing on the specification rather than on the data-generation.

Property-Based Testing

Property-based testing allows to formulate *functional specifications* in code which then a property-based testing library tries to falsify by *automatically* generating test-data, covering as much cases as possible. When a case is found for which the property fails, the library then reduces the test-data to its simplest form for which the test still fails e.g. shrinking a list to a smaller size. It is clear to see that this kind of testing is especially suited to ABS, because we can formulate specifications, meaning we describe *what* to test instead of *how* to test. Also the deductive nature of falsification in property-based testing suits very well the constructive and exploratory nature of ABS. Further, the automatic test-generation can make testing of large scenarios in ABS feasible because it does not require the programmer to specify all test-cases by hand, as is required in e.g. traditional unit tests.

Property-based testing was introduced in [31, 32] where the authors present the QuickCheck library in Haskell, which tries to falsify the specifications by *randomly* sampling the test space. We argue, that the stochastic sampling nature of this approach is particularly well suited to ABS, because it is itself almost always driven by stochastic events and randomness in the agents behaviour, thus this correlation should make it straightforward to map ABS to property-testing. According to the authors of QuickCheck *"The major limitation is that there is no measurement of test coverage."* [31]. Although QuickCheck provides help to report the distribution of test-cases it is not able to measure the coverage of tests in general. This could lead to the case that test-cases which would fail are never tested because of the stochastic nature of QuickCheck. Fortunately, the library provides mechanisms for the developer to measure coverage in specific test-cases where the data and its (expected) distribution is known to the developer. This is a powerful tool for testing randomness in ABS as will be shown in subsequent chapters.

As a remedy for the potential coverage problems of QuickCheck, there exists also a deterministic property-testing library called SmallCheck [133], which instead of randomly sampling the test-space, enumerates test-cases exhaustively up to some depth. It is based on two observations, derived from model-checking, that (1) *"If a program fails to meet its specification in some cases, it almost always fails in some simple case"* and (2) *"If a program does not fail in any simple case, it hardly ever fails in any case* [133]. This non-stochastic approach to property-based testing might be a complementary addition in some cases where the tests are of non-stochastic nature with a search-space too large to test manually by unit tests but small enough to enumerate exhaustively. The main difficulty and weakness of using SmallCheck is to reduce the dimensionality of the test-case depth search to prevent combinatorial explosion, which

would lead to exponential number of cases. Thus one can see QuickCheck and SmallCheck as complementary instead of in opposition to each other.

A brief overview of QuickCheck

To give a good understanding on how property-based testing works with QuickCheck, we give a few examples of property-tests on lists, which are directly expressed as functions in Haskell. Such a function has to return a *Bool* which indicates *True* in case the test succeeds or *False* if not and can take input arguments which data is automatically generated by QuickCheck.

```
-- append operator (++) is associative
append_associative :: [Int] -> [Int] -> [Int] -> Bool
append_associative xs ys zs = (xs ++ ys) ++ zs == xs ++ (ys ++ zs)

-- The reverse of a reversed list is the original list
reverse_reverse :: [Int] -> Bool
reverse_reverse xs = reverse (reverse xs) == xs

-- reverse is distributive over append (++)
-- This test fails for explanatory reasons, for a correct
-- property xs and ys need to be swapped on the right-hand side!
reverse_distributive :: [Int] -> [Int] -> Bool
reverse_distributive xs ys = reverse (xs ++ ys) == reverse xs ++ reverse ys

-- running the tests
main :: IO ()
main = do
  quickCheck append_associative
  quickCheck reverse_reverse
  quickCheck reverse_distributive
```

When we run the tests using *main*, we get the following output:

```
+++ OK, passed 100 tests.
+++ OK, passed 100 tests.
*** Failed! Falsifiable (after 5 tests and 6 shrinks):
[0]
[1]
```

We see that QuickCheck generates 100 test-cases for each property-test and it does this by generating random data for the input arguments. Note that we have not specified any data for our input arguments; QuickCheck is able to provide a suitable data-generator through type-inference: for lists and all the existing Haskell types there exist custom data-generators already.

QuickCheck generates 100 test-cases by default and requires all to pass - if there is a test-case which fails, the overall property-test fails and QuickCheck shrinks the input to a minimal size which still fails and reports it as a counter example. This is the case in the last property-test *reverse_distributive* which is wrong as *xs* and *ys* need to be swapped on the right-hand side. In this run, QuickCheck found a counter-example to the property after 5 tests and applied

6 shrinks to find the minimal failing example of *xs = [0]* and *ys = [1]*. If we swap *xs* and *ys*, the property-test passes 100 test-cases just like the other two did. Note that it is possible to configure QuickCheck to generate more or less random test-cases, which can be used to increase the coverage if the sampling space is quite large - this will become useful later.

Generators

QuickCheck comes with a lot of data-generators for existing types like Strings, Int, Double, Lists,... but in case one wants to randomize custom data-types one has to write custom data-generators. There are two ways to do this: fix them at compile-time by writing an *Arbitrary* instance or write a run-time generator running in the *Gen* Monad. The advantage of having an *Arbitrary* instance is that the custom data-type can then be used as random argument to a function as in the examples above.

Lets implement a custom data-generator for the *SIRState* for both cases. Lets start with the run-time option, running in the *Gen* Monad:

```
genSIRState :: Gen SIRState
genSIRState = elements [Susceptible, Infected, Recovered]
```

This implementation makes use of the *elements :: [a] → Gen a* functions, which picks a random element from a non-empty list with uniform probability. If a skewed distribution is needed, one can use the *frequency :: [(Int, Gen a)] → Gen a* function, where a frequency can be specified for each element. For example to generate on average 80% Susceptible, 15% Infected and 5% Recovered can be achieved using this function:

```
genSIRState :: Gen SIRState
genSIRState = frequency [(80, Susceptible), (15, Infected), (5, Recovered)]
```

Implementing an *Arbitrary* instance is straight forward, one only needs to implement the *arbitrary :: Gen a* method:

```
instance Arbitrary SIRState where
  arbitrary = genSIRState
```

When we have a random Double as input to a function but want to restrict its random range to (0,1) because it reflects a probability, we can do this easily with *newtype* and implementing an *Arbitrary* instance. The same can be done for limiting the simulation duration to a lower range than the full Double range.

```
newtype Probability = P Double deriving Show
newtype TimeRange   = T Double deriving Show

instance Arbitrary Probability where
  arbitrary = P <$> choose (0, 1)

instance Arbitrary TimeRange where
  arbitrary = T <$> choose (0, 50)
```

The simulations we run all rely on a random-number generator, thus we need a randomly initialised random-number generator each time we run a simulation. This can be easily achieved by drawing a seed from the full Int range and creating an *StdGen* from it:

```
genStdGen :: Gen StdGen
genStdGen = mkStdGen <$> choose (minBound, maxBound)

instance Arbitrary StdGen where
  arbitrary = genStdGen
```

This generator then can be used to write another custom data-generator which generates simulation runs. Here we give an example for the time-driven SIR:

```
genTimeSIR :: [SIRState]   -- ^ Population
           -> Double       -- ^ Contact rate
           -> Double       -- ^ Infectivity
           -> Double       -- ^ Illness duration
           -> Double       -- ^ Time Delta
           -> Double       -- ^ Time Limit
           -> Gen [(Double, (Int, Int, Int))]
genTimeSIR as cor inf ild dt tMax
  = runTimeSIRFor as cor inf ild dt tMax <$> genStdGen
```

Distributions

As already mentioned, QuickCheck provides functions to measure the coverage of test-cases. This can be done using the *label :: Testable prop* $\Rightarrow$ *String* $\rightarrow$ *prop* $\rightarrow$ *Property* function. It takes a *String* as first argument and a testable property and constructs a *Property*. QuickCheck collects all generated labels, counts their occurrences and reports their distribution. For example it could be used to get a rough idea about the length of the random lists created in the *reverse_reverse* property shown above:

```
reverse_reverse_label :: [Int] -> Property
reverse_reverse_label xs
  = label ("length of random-list is " ++ show (length xs))
          (reverse (reverse xs) == xs)
```

When running the test, we see the following output:

```
+++ OK, passed 100 tests:
 5% length of random-list is 27
 5% length of random-list is 15
 5% length of random-list is 0
 4% length of random-list is 4
 4% length of random-list is 19
 ...
```

Coverage

The most powerful functions to work with test-case distributions though are *cover* and *checkCoverage*. The function *cover :: Testable prop ⇒ Double → Bool → String → prop → Property* allows to explicitly specify that a given percentage of successful test-cases belong to a given class. The first argument is the expected percentage, the second argument is a *Bool* which indicates whether the current test-case belongs to the class or not; the third argument is a label for the coverage; the fourth argument is the property which needs to hold for the test-case to succeed.

Lets look at an example - we use *cover* to express that we expect 15% of all test-cases to have a random list with at least 50 elements.

```
reverse_reverse_cover :: [Int] -> Property
reverse_reverse_cover xs
  = cover 15 (length xs >= 50) "Length of random-list at least 50"
             (reverse (reverse xs) == xs)
```

When repeatedly running the test, we see the following output:

```
+++ OK, passed 100 tests (10% length of random-list at least 50).
Only 10% Length of random-list at least 50, but expected 15%.
+++ OK, passed 100 tests (21% length of random-list at least 50).
```

As can be seen, QuickCheck runs the default 100 test-cases and prints a warning if the expected coverage is not reached. This is quite nice but it is up to us to decide whether 100 test-cases are suitable and whether we can really claim that the given coverage will be reached or not. Fortunately, QuickCheck provides the powerful function *checkCoverage :: Testable prop ⇒ prop → Property* which does this for us. When *checkCoverage* is used, QuickCheck will run an increasing number of test-cases until it can decide whether the percentage in *cover* was reached or cannot be reached at all. The way QuickCheck does it, is by using sequential statistical hypothesis testing [160], thus if QuickCheck comes to the conclusion that the given percentage can or cannot be reached, it is based on a robust statistical test giving strong confidence in the result.

When we run the example from above but now with *checkCoverage* we get the following output:

```
+++ OK, passed 12800 tests
    (15.445% length of random-list at least 50).
```

We see that after QuickCheck has ran 12,800 tests it came to the statistically robust conclusion that indeed at least 15% of the test-cases have a random-list with at least 50 elements.

Emulating Failure

As already mentioned, *all* test-cases have to pass for the whole property-test to succeed. If just a single test-case fails, the whole property-test fails. This is

sometimes too strong, especially when we are dealing with stochastic systems like ABS models.

The function *cover* can be used to emulate failure of test-cases and get a measure of failure. Instead of computing the *True/False* property in the last *prop* argument, we set the last argument always to *True* and compute the *True/False* property in the second *Bool* argument. This has the effect that *all* test-cases are successful but that we get a distribution of failed/successful ones. In combination with *checkCoverage*, this is a particularly powerful pattern for testing ABS which allows us to test hypotheses and statistical tests on distributions as will be shown in later chapters.

Chapter 9

Testing Agent specifications

In this chapter we are showing how to use QuickCheck to encode full agent-specifications directly in code as property-tests. These properties serve then both as formal specification and tests at the same time - a fundamental strength of property-based testing, not possible with unit-testing in this strong expressive form. Besides the high expressivity, QuickCheck also allows us to state statistical coverage for certain cases, which allows to express statistical properties of the agents behaviour, something also not directly possible with unit-testing. This is a very strong indication that property-based testing is a natural fit to test agent-based simulation. We discuss both time- and event-driven implementations of the agent-based SIR model as introduced in Chapter 2.2.1.

9.1 Event-Driven specification

In this section we present how QuickCheck can be used to test event-driven agents by expressing their *specification* as property-tests in the case of the event-driven SIR implementation from chapter 5.2.

In general, testing event-driven agents is fundamentally different and more complex than testing time-driven agents, as their interface surface is generally much larger: events form the input to the agents to which they react with new events - the dependencies between those can be quite complex and deep. Using property-based tests we can encode the invariants and end up with an actual specification of their behaviour, acting as documentation, regression test within a TDD and property tests.

Note that the concepts presented here are applicable with slight adjustments to the Sugarscape implementation as well but we focused on the SIR one as its specification is shorter and does not require as much in-depth details - after all we are interested in deriving concepts, not dealing with specific technicalities.

With event-driven ABS a good starting point in specifying and then testing the system is simply relating the input events to expected output events. In the SIR implementation we have only 3 events, making it feasible to give a full

formal specification - note that the Sugarscape implementation has more than 16 events, which makes it much harder to test it with sufficient coverage, giving a good reason to primarily focus on the SIR implementation.

9.1.1 Deriving the specification

We start by giving the full *specification* of the susceptible, infected and recovered agent by stating the input-to-output event relations. The susceptible agent is specified as follows:

1. *MakeContact* - If the agent receives this event it will output β *Contact ai Susceptible* events, where ai is the agents self id. The events have to be scheduled immediately without delay, thus having the current time as scheduling time-stamp. The receivers of the events are uniformly randomly chosen from the agent population. The agent doesn't change its state, stays *Susceptible* and does not schedule any other events than the ones mentioned.

2. *Contact _ Infected* - If the agent receives this event there is a chance of uniform probability γ (infectivity) that the agent becomes *Infected*. If this happens, the agent will schedule a *Recover* event to itself into the future, where the time is drawn randomly from the exponential distribution with $\lambda = \delta$ (illness duration). If the agent does not become infected, it won't change its state, stays *Susceptible* and does not schedule any events.

3. *Contact _ _* or *Recover* - If the agent receives any of these (other) events it won't change its state, stays *Susceptible* and does not schedule any events.

This specification implicitly covers that a susceptible agent can never transition from a *Susceptible* to a *Recovered* state within a single event - it can only make the transition to *Infected* or stays *Susceptible*. The infected agents are specified as follows:

1. *Recover* - If the agent receives this, it will not schedule any events and make the transition to the *Recovered* state.

2. *Contact sender Susceptible* - If the agent receives this, it will reply immediately with *Contact ai Infected* to *sender*, where *ai* is the infected agents id and the scheduling time-stamp is the current time. It will not schedule any events and stays *Infected*.

3. In case of any other event, the agent will not schedule any events and stays *Infected*.

This specification implicitly covers that an infected agent never goes back to the *Susceptible* state - it can only make the transition to *Recovered* or stay *Infected*. From the specification of the susceptible agent it becomes clear that a

susceptible agent who became infected, will always recover as the transition to *Infected* includes the scheduling of *Recovered* to itself.

The *recovered* agents specification is very simple. It stays *Recovered* forever and does not schedule any events.

The question is now how to put these into a property-test with QuickCheck. We focus on the susceptible agent, as it it the most complex one, which concepts can then be easily applied to the other two. Generally speaking, we create a random *susceptible* agent and a random event, feed it to the agent to get the output and check the invariants accordingly to input and output.

9.1.2 Encoding invariants

We start by encoding the invariants of the susceptible agent directly into Haskell, implementing a function which takes all necessary parameters and returns a *Bool* indicating whether the invariants hold or not. The encoding is straightforward when using pattern matching and it nearly reads like a formal specification due to the declarative nature of functional programming.

```
susceptibleProps :: SIREvent              -- ^ Random event sent to agent
                 -> SIRState              -- ^ Output state of the agent
                 -> [QueueItem SIREvent]  -- ^ Events the agent scheduled
                 -> AgentId               -- ^ Agent id of the agent
                 -> Bool
-- received Recover => stay Susceptible, no event scheduled
susceptibleProps Recover Susceptible es _ = null es
-- received MakeContact => stay Susceptible, check events
susceptibleProps MakeContact Susceptible es ai
  = checkMakeContactInvariants ai es cor
-- received Contact _ Recovered => stay Susceptible, no event scheduled
susceptibleProps (Contact _ Recovered) Susceptible es _ = null es
-- received Contact _ Susceptible => stay Susceptible, no event scheduled
susceptibleProps (Contact _ Susceptible) Susceptible es _  = null es
-- received Contact _ Infected, didn't get Infected, no event scheduled
susceptibleProps (Contact _ Infected) Susceptible es _ = null es
-- received Contact _ Infected AND got infected, check events
susceptibleProps (Contact _ Infected) Infected es ai
  = checkInfectedInvariants ai es
-- all other cases are invalid and result in a failed test-case
susceptibleProps _ _ _ _ = False
```

Next we give the implementation for the *checkMakeContactInvariants* and *checkInfectedInvariants* functions. The function *checkMakeContactInvariants* encodes the invariants which have to hold when the susceptible agent receives a *MakeContact* event. The *checkInfectedInvariants* function encodes the invariants which have to hold when the susceptible agent got *Infected*. Both implementations reads like a formal specification, again thanks to the declarative nature of functional programming and pattern matching:

```
checkInfectedInvariants :: AgentId              -- ^ Agent id of the agent
                        -> [QueueItem SIREvent] -- ^ Events the agent scheduled
                        -> Bool
```

```
checkInfectedInvariants sender
  -- expect exactly one Recovery event
  [QueueItem receiver (Event Recover) t']
  -- receiver is sender (self) and scheduled into the future
  = sender == receiver && t' >= t
-- all other cases are invalid
checkInfectedInvariants _ _ = False
```

The *checkMakeContactInvariants* is a bit more complex but reads as a formal specification as well:

```
checkMakeContactInvariants :: AgentId              -- ^ Agent id of the agent
                           -> [QueueItem SIREvent] -- ^ Events the agent scheduled
                           -> Int                  -- ^ Contact Rate
                           -> Bool
checkMakeContactInvariants sender es contactRate
    -- make sure there has to be exactly one MakeContact event and
    -- exactly contactRate Contact events
    = invOK && hasMakeCont && numCont == contactRate
  where
    (invOK, hasMakeCont, numCont)
      = foldr checkMakeContactInvariantsAux (True, False, 0) es

    checkMakeContactInvariantsAux :: QueueItem SIREvent
                                  -> (Bool, Bool, Int)
                                  -> (Bool, Bool, Int)
    checkMakeContactInvariantsAux
        (QueueItem receiver (Event (Contact sender' Susceptible)) t') (b, mkb, n)
      = (b && sender == sender'    -- the sender in Contact must be the Susceptible agent
           && receiver `elem` ais  -- the receiver of Contact must be in the agent ids
           && t == t', mkb, n+1)   -- the Contact event is scheduled immediately
    checkMakeContactInvariantsAux
        (QueueItem receiver (Event MakeContact) t') (b, mkb, n)
      = (b && receiver == sender   -- the receiver of MakeContact is the Susceptible agent itself
           && t' == t + 1.0        -- the MakeContact event is scheduled 1 time-unit into the future
           &&  not mkb, True, n)   -- there can only be one MakeContact event
    checkMakeContactInvariantsAux _ (_, _, _)
      = (False, False, 0) -- other patterns are invalid
```

What is left is to actually write a property-test using QuickCheck. We are making heavy use of random parameters to express that the properties have to hold invariant of the model parameters. We make use of additional data-generator modifiers: *Positive* ensures that the value generated is positive; *NonEmptyList* ensures that the randomly generated list is non-empty.

```
prop_susceptible_invariants :: Positive Int         -- ^ Contact rate
                            -> Probability          -- ^ Infectivity
                            -> Positive Double      -- ^ Illness duration
                            -> Positive Double      -- ^ Current simulation time
                            -> NonEmptyList AgentId -- ^ Agent ids of the population
                            -> Gen Property
prop_susceptible_invariants
  (Positive cor) (P inf) (Positive ild) (Positive t) (NonEmpty ais) = do
  -- generate random event, requires the population agent ids
  evt <- genEvent ais
  -- run susceptible random agent with given parameters
```

```
(ai, ao, es) <- genRunSusceptibleAgent cor inf ild t ais evt
-- check properties
return $ property $ susceptibleProps evt ao es ai
```

When running this property-test all 100 test-cases pass. Due to the large random sampling space with 5 parameters, we increase the number of test-cases to generate to 100,000 - still all test-cases pass.

9.1.3 Encoding transition probabilities

In the specifications above there are probabilistic state-transitions, for example an infected agent *will* recover after a given time, which is randomly distributed with the exponential distribution. The susceptible agent *might* become infected, depending on the events it receives and the infectivity (γ) parameter. We look now into how we can encode these probabilistic properties using the powerful *cover* and *checkCoverage* feature of QuickCheck.

9.1.3.1 Susceptible agent

We follow the same approach as in encoding the invariants of the susceptible agent but instead of checking the invariants, we compute the probability for each case. Note that in this property-test we cannot randomise the model parameters because this would lead to random coverage. This might seem like a disadvantage but we do not really have a choice here - still, the model parameters can be adjusted arbitrarily and the property (must) still hold. We make use of the *cover* function together with *checkCoverage*, which ensures that we get a statistical robust estimate whether the expected percentages can be reached or not. Implementing this property-test is then simply a matter of computing the probabilities and of case analysis over the random input event and the agents output.

```
...
case evt of
  Recover ->
    cover recoverPerc True
     ("Susceptible receives Recover, expected " ++ show recoverPerc) True
...
```

Note the usage pattern of *cover*: we always include the test-case into the coverage class and all test-cases pass. The reason for this is that we are just interested in testing the coverage, which is in fact the property we want to test. We could have combined this test into the previous one but then we couldn't have use randomised model parameters. For this reason, and to keeps the concerns separated we opted for two different tests, which makes them also much more readable.

When running the property-test we get the following output:

```
+++ OK, passed 819200 tests:
33.3582% Susceptible receives MakeContact, expected 33.33%
```

```
33.2578% Susceptible receives Recover, expected 33.33%
11.1643% Susceptible receives Contact * Recovered, expected 11.11%
11.1096% Susceptible receives Contact * Susceptible, expected 11.11%
10.5616% Susceptible receives Contact * Infected, stays Susceptible, expected 10.56%
 0.5485% Susceptible receives Contact * Infected, becomes Infected, expected 0.56%
```

After 819,200 (!) test-cases QuickCheck comes to the conclusion that the distributions generated by the test-cases reflect the expected distributions and passes the property-test. We see that the values do not match exactly in some cases but by using sequential statistical hypothesis testing QuickCheck is able to conclude that the coverage are statistically equal.

9.1.3.2 Infected agent

We want to write a property-test which checks whether the transition from *Infected* to *Recovered* actually follows the exponential distribution with a fixed δ (illness duration). The idea is to compute an expected probability agents have an illness duration of less or equal δ. This probability is given by the cumulative density function (CDF) of the exponential distribution. The question is how to get the infected illness duration. This is simply achieved by infecting a susceptible agent and taking the scheduling time of the *Recover* event. We have written a custom data-generator for this:

```haskell
getInfectedAgentDuration :: Double -> Gen (SIRState, Double)
getInfectedAgentDuration ild = do
  -- with these parameters the susceptible agent WILL become infected
  (_, ao, es) <- genRunSusceptibleAgent 1 1 ild 0 [0] (Contact 0 Infected)
  return (ao, recoveryTime es)
  where
    -- expect exactly one event: Recover
    recoveryTime :: [QueueItem SIREvent] -> Double
    recoveryTime [QueueItem _ (Event Recover) t]  = t
    recoveryTime _ = 0
```

Encoding the probability check into a property-test is straight-forward:

```haskell
prop_infected_duration :: Property
prop_infected_duration = checkCoverage (do
  -- fixed model parameter, otherwise random coverage
  let ild  = 15
  -- compute probability drawing a random value less or equal
  -- ild from the exponential distribution (follows the CDF)
  let prob = 100 * expCDF (1 / ild) ild

  -- run random susceptible agent to become infected and
  -- return agents state and recovery time
  (ao, dur) <- getInfectedAgentDuration ild

  return (cover prob (dur <= ild)
            ("Infected agent recovery time is less or equals " ++ show ild ++
             ", expected at least " ++ show prob)
            (ao == Infected)) -- final state has to Infected
```

When running the property-test we get the following output.

```
+++ OK, passed 3200 tests
    (63.62% Infected agent recovery time is less or equals 15.0,
     expected at least 63.21%).
```

QuickCheck is able to determine after only 3,200 test-cases that the expected coverage is met and passes the property-test.

9.2 Time-driven specification

The time-driven SIR agents have a very small interface: they only receive the agent-population from the previous step and output their state in the current step. We can also assume an implicit forward flow of time, statically guaranteed by Yampas arrowized FRP. Thus a specification in time-driven approach is given in terms of probabilities and timeouts, rather than in events as in the event-driven testing as presented before.

- Susceptible agent - makes *on average* contact with β (contact rate) agents per time-unit. The distribution follows the exponential distribution with $\lambda = \frac{1}{\beta}$. If a susceptible agents get into contact with an infected agent, it will become infected with a uniform probability of γ (infectivity).
- Infected agent - *will* recover *on average* after δ (illness duration) time units. The distribution follows the exponential distribution with $\lambda = \delta$.
- Recovered agent - stays recovered *forever*.

9.2.1 Specifications of the susceptible agent

We cannot directly observe that a susceptible agent makes contact with other agents like we can in the event-driven approach but only indirectly through its change of state: a susceptible agent *might* become infected if there are infected agents in the population. Thus when we run a susceptible agent for some time, we have 3 possible outcomes of the agents output stream: 1. the agent did not get infected and thus all elements of the stream are *Susceptible*; 2. the agent got infected thus up to a given index in the stream all elements are *Susceptible* and change to *Infected* after; 3. the agent got *Infected* and then *Recovered* thus the stream is the same as in infected but there is a second index after which all elements change to *Recovered*. Encoding them in code is straightforward:

```
susceptibleInvariants :: [SIRState] -- ^ The output stream of the susceptible agent
                      -> Bool       -- ^ The population contains an infected agent
                      -> Bool       -- ^ True in case the invariant holds
susceptibleInvariants aos infInPop
    -- Susceptible became Infected and then Recovered
    | isJust recIdxMay
      = infIdx < recIdx &&  -- agent has to become infected before recovering
        all (==Susceptible) (take infIdx aos) &&
        all (==Infected) (take (recIdx - infIdx) (drop infIdx aos)) &&
        all (==Recovered) (drop recIdx aos) &&
```

```
        infInPop  -- can only happen if there are infected in the population

    -- Susceptible became Infected
    | isJust infIdxMay
      = all (==Susceptible) (take infIdx aos) &&
        all (==Infected) (drop infIdx aos) &&
        infInPop -- can only happen if there are infected in the population

    -- Susceptible stayed Susceptible
    | otherwise = all (==Susceptible) aos
  where
    -- look for the first element when agent became Infected
    infIdxMay = elemIndex Infected aos
    -- look for the first element when agent became Recovered
    recIdxMay = elemIndex Recovered aos

    infIdx = fromJust infIdxMay
    recIdx = fromJust recIdxMay
```

Putting this into a property-test is also straightforward. We generate a random population, run a random susceptible agent with a sampling rate of $\Delta t = 0.01$ and check the invariants on its output stream. These invariants all have to hold independently from the (positive) duration we run the random susceptible agent for, thus we run it for a random amount of time units. The invariants also have to hold for arbitrary positive beta (contact rate), gamma (infectivity) and delta (illness duration). At the same time, we want to get an idea of the percentage of agents which stayed susceptible, became infected or made the transition to recovered, thus we *label* all our test-cases accordingly.

```
prop_susceptible_invariants :: Positive Double  -- ^ beta, contact rate
                            -> Probability      -- ^ gamma, infectivity within (0,1) range
                            -> Positive Double  -- ^ delta, illness duration
                            -> TimeRange        -- ^ simulation duration, within (0,50) range
                            -> [SIRState]       -- ^ population
                            -> Property
prop_susceptible_invariants
      (Positive cor) (P inf) (Positive ild) (T t) as = property (do
    -- population contains an infected agent True/False
    let infInPop = Infected `elem` as

    -- run a random susceptible agent for random time-units with
    -- sampling rate dt 0.01 and return its stream of output
    aos <- genSusceptible cor inf ild as t 0.01

    return
        -- label all test-cases
        label (labelTestCase aos)
        -- check invariants on output stream
        (property (susceptibleInvariants aos infInPop))
  where
    labelTestCase :: [SIRState] -> String
    labelTestCase aos
      | Recovered `elem` aos = "Susceptible -> Infected -> Recovered"
      | Infected `elem` aos  = "Susceptible -> Infected"
      | otherwise            = "Susceptible"
```

Due to the high dimensionality of the random sampling space, we run 10,000 tests - all succeed as expected.

```
SIR Agent Specifications Tests
  Susceptible agents invariants: OK (12.72s)
    +++ OK, passed 10000 tests:
    55.78% Susceptible -> Infected -> Recovered
    37.19% Susceptible -> Infected
     7.03% Susceptible
```

This test so far did not state anything about the probability of a susceptible agent getting infected. The probability for it is bimodal (see Chapter 11) due to the combined probabilities of the exponential distribution of the contact rate and the uniform distribution of the infectivity. Unfortunately, the bimodality makes it not possible to compute a coverage percentage of infected in this case, as we did in the event-driven test because the bimodal distribution can only be described in terms of a distribution and not a single probability. This was possible in the even-driven approach because we decoupled the production of the *Contact _ Infected* event from the infection: both were uniform distributed, thus we could compute a coverage percentage. Thus we see that different approaches also allow different explicitness of testing.

9.2.2 Probabilities of the infected agent

An infected agent *will* recover after *finite* time, thus we assume that there exists an index in the output stream, where the elements will change to *Recovered*. From the index we can compute the time of recovery, knowing the fixed sampling rate Δt.

```
infectedInvariant :: [SIRState]      -- ^ The stream of outputs from the infected agent
                  -> Double          -- ^ Sampling rate dt
                  -> Maybe Double    -- ^ Just recovery time, or Nothing if not recovered
infectedInvariant aos dt  = do
  -- search for the index of the first Recovery element
  recIdx <- elemIndex Recovered aos
  -- all elements up to the index need to be Infected,
  -- because the agent cannot go back to Susceptible
  if all (==Infected) (take recIdx aos)
    then Just (dt * recIdx)
    else Nothing
```

To put this into a property-test, we follow a similar approach as in the event-driven case of the infected agents invariants. We employ the CDF of the exponential distribution to get the probability of an agent recovering within δ (illness duration) time steps. We then run a random infected agent for an *unlimited* time with a sampling rate o f $\Delta t = 0.01$ and search in its potentially infinite output stream for the first occurrence of an *Infected* element to compute the recovery time, as shown in the invariant above. The code is conceptually exactly the same as in the event-driven case, so we do not repeat the property-test here.

When running the test we get the following output, indicating that QuickCheck finds the coverage satisfied after 3,200 test-cases:

```
+++ OK, passed 3200 tests (62.28% infected agents have an illness
    duration of 15.0 or less, expected 63.21).
```

The fact that we run the random infected agent without time-limit explicitly expresses the invariant that an infected agent *will* recover in *finite* time-steps: a correct implementation will produce a stream which contains an index from which on elements are all *Infected*, thus resulting in *Just* recovery time. This is a direct expression of the fact that the CDF of the exponential distribution reaches 100% at infinity. An approach which would guarantee the termination would be to limit the time to run the infected agent to *illnessDuration* and evaluate the property always to True. This approach guarantees termination but removes an important part of the specification - we decided to follow the initial approach to make the specification really clear, and in practice it has turned out to terminate within a very short time (see below).

9.2.3 The non-computability of the recovered agent test

The property-test for the recovered agent is trivial: we run a random recovered agent for a random number of time-units with $\Delta t = 0.01$ and require that all elements in the output stream are *Recovered*. Of course this is no proof that the recovered agent stays recovered *forever* as this would take *forever* to test and is thus not computable. Here we are hitting the limits of what is possible with random black-box testing: without looking at the actual implementation it is not possible to prove that the recovered agent is really behaving as specified. We made this fact very clear at the beginning of this thesis part: property-based testing is not a proof for the correctness but only supports one in raising the confidence in the correctness by constructing cases which show that the behaviour is not incorrect.

To be really sure that the recovered agent behaves as specified we need to employ white-box verification and look at the actual implementation. It is immediately obvious that the implementation follows the specification and actually *is* the specification, and we can even regard it as a very concise proof that it will stay recovered *forever*:

```
recoveredAgent :: SIRAgent
recoveredAgent = constant Recovered
```

The signal function *constant* is the *const* function lifted into an arrow: *constant b = arr (const b)*. This should be proof enough that a recovered agent will stay recovered *forever*. We discuss this the topic of computability in pure functional ABS in a slightly different context in Appendix B.

9.3 Discussion

In this section we have shown how to express the specifications of both the event- and time-driven agent behaviour directly in code as properties and how to implement property-tests in QuickCheck for them. The approach to event-driven properties was to establish a correspondence between an input-event the current agent-state and the output events and the new agents state. In case of the time-driven agent, the properties are expressed in terms of a potentially infinite stream of agent output-states. Although both implementations follow the same underlying model, the technical details of the properties differ substantially. The reason for this is that although property-based testing is a black-box verification technique, the implementation often requires substantial knowledge of the internal details as can be seen especially in the event-driven case.

The resulting properties are highly expressive due to pattern matching and declarative programming and can be regarded as a kind of formal specification. Together with the properties which check the state-transition probabilities, we claim that the property-tests shown in this chapter fully specify both the event- and time-driven agent behaviour. This is a first example emphasising the usefulness of QuickCheck for testing ABS, providing a first strong evidence for the hypothesis that randomised property-testing is a good match for testing ABS.

Curiously, the implementation of all the specifications and property-tests is a lot larger than the original implementations. Still, that is not the point here: we showed how to implement a full specification of an ABS model as a property-based test and we succeeded! This is definitely a strong indication that our hypothesis that randomised property-based testing is a suitable tool for testing ABS is valid. With unit tests we would be quite lost here: even for the SIR model, it is hard to enumerate all possible interactions and cases but by stating invariants as properties and generating random test-cases we make sure they are checked.

We have not looked into more complex testing patterns like the synchronous agent-interactions of Sugarscape. We didn't look into testing full agent and interacting agent behaviour using property-tests due to its complexity which would justify a part paper alone. Due to its inherent stateful nature with complex dependencies between valid states and agents actions we need a more sophisticated approach as outlined in [41], where the authors show how to build a meta-model and commands which allow to specify properties and valid state-transitions which can be generated automatically. We leave this for further research.

What is particularly powerful is that one has complete control and insight over the changed state before and after e.g. a function was called on an agent: thus it is very easy to check if the function just tested has changed the agent-state itself or the environment: the new environment is returned after running the agent and can be checked for equality of the initial one - if the environments are not the same, one simply lets the test fail. This behaviour is very hard to emulate in OOP because one can not exclude side-effect at compile time, which

means that some implicit data-change might slip away unnoticed. In FP we get this for free.

Note that by exploiting lazy evaluation in the time-driven tests we scratch on what is conveniently possible in established approaches to ABS: we can let the simulation run potentially forever as in the case of the infected agent and rely on the correctness of the implementation to terminate in finite step when consuming the potentially infinite stream.

Note that we did not include an explicit environment in our agent specification tests and assumed a full connected network where all agents can make contact with each other. We think that property-based testing is highly useful there as well, especially when dealing with random environment like in Sugarscape or social and random networks [87, 46]. We leave this for further research but we hypothesise that for the SIR model all properties presented here should still hold under different environments.

Chapter 10

Testing SIR Invariants

The tests in the previous chapter were stateless: only one computational step of an agent was considered by feeding a single event and ignoring the agent continuation. Also the events didn't contain any notion of time as they would carry within the queue. Feeding follow-up events into the continuation would make testing inherently stateful as we introduce history into the system. Such tests would allow to test the full life-cycle of one agent or a full population.

In this chapter we will discuss how we can encode properties and specifications which require stateful testing. We define stateful testing here as: evolving a simulation state consisting of one or more agents over multiple events. Note that this also includes running the whole simulation. Note that we primarily focus on the event-driven implementation here unless noted otherwise.

We first show how we can encode actual laws of the underlying SIR model into properties and write property-tests in QuickCheck for them. We then employ random event-sampling to check whether these invariants also hold when ignoring the event-interdependencies between agents. Finally we compare both the event- and time-driven implementations with each other, giving an excellent use-case for property-based testing in ABS.

10.1 Deriving the invariants

By informally reasoning about the agent specification and by realising that they are in fact a state-machine with a one-directional flow of *Susceptible* $\rightarrow$ *Infected* $\rightarrow$ *Recovered*, we can come up with a few invariants which have to hold for any SIR simulation run independent of the random-number stream and the population:

1. Simulation time is monotonic increasing. Each event carries a time-stamp when it is scheduled. This time-stamp may stay constant between multiple events but will eventually increase and must never decrease. Obviously this invariant is a fundamental assumption in most simulations: time advances into the future and does not flow backwards.

2. The number of total agents N stays constant. The SIR model does not specify the dynamic creation or removal of agents during simulation. This is in contrast to the Sugarscape where, depending on the model parameters, this can be very well the case.

3. The number of *Susceptible* agents S is monotonic decreasing. Susceptile agents *might* become infected, reducing the total number of susceptible agents but they can never increase because neither an infected nor recovered agent can go back to *Susceptible*.

4. The number of *Recovered* agents R is monotonic increasing. This is because infected agents *will* recover, leading to an increase of recovered agents but once the recovered state is reached, there is no escape from it.

5. The number of *Infected* agents respects the invariant of the equation $I = N - (S + R)$ for every step. This follows directly from the first property which says $N = S + I + R$.

10.2 Encoding the invariants

All of those properties are easily expressed directly in code and read like a formal specification due to the declarative nature of functional programming:

```
sirInvariants :: Int                        -- ^ N total number of agents
              -> [(Time,(Int,Int,Int))] -- ^ simulation output for each step/event: (Time, (S,I,R))
              -> Bool
sirInvariants n aos = timeInc && aConst && susDec && recInc && infInv
  where
    (ts, sirs)  = unzip aos
    (ss, _, rs) = unzip3 sirs

    -- 1. time is monotonic increasing
    timeInc = allPairs (<=) ts
    -- 2. number of agents N stays constant in each step
    aConst = all agentCountInv sirs
    -- 3. number of susceptible S is monotonic decreasing
    susDec = allPairs (>=) ss
    -- 4. number of recovered R is monotonic increasing
    recInc = allPairs (<=) rs
    -- 5. number of infected I = N - (S + R)
    infInv = all infectedInv sirs

    agentCountInv :: (Int,Int,Int) -> Bool
    agentCountInv (s,i,r) = s + i + r == n

    infectedInv :: (Int,Int,Int) -> Bool
    infectedInv (s,i,r) = i == n - (s + r)

    allPairs :: (Ord a, Num a) => (a -> a -> Bool) -> [a] -> Bool
    allPairs f xs = all (uncurry f) (pairs xs)
```

```
    pairs :: [a] -> [(a,a)]
    pairs xs = zip xs (tail xs)
```

Putting this property into a QuickCheck test is straightforward. Note that we use randomise the model parameters β (contact rate), γ (infectivity) and δ (illness duration) because the properties have to hold for all positive, finite model parameters.

```
prop_sir_invariants :: Positive Int     -- ^ beta, contact rate
                    -> Probability      -- ^ gamma, infectivity in range (0,1)
                    -> Positive Double  -- ^ delta, illness duration
                    -> TimeRange        -- ^ random duration in range (0, 50)
                    -> [SIRState]       -- ^ population
                    -> Property
prop_sir_invariants
    (Positive cor) (P inf) (Positive ild) (T t) as  = property (do
  -- total agent count
  let n = length ss
  -- run the SIR simulation with a new RNG
  ret <- genSimulationSIR ss cor inf ild t
  -- check invariants and return result
  return (sirInvariants n ret)
```

Due to the large sampling space, we increase the number of test-cases to run to 10,000 and unsurprisingly all tests pass. Note that we put a random time-limit of (0,50) on the simulations to run, meaning that if a simulation does not terminate before that limit, it will be terminated at that random t. This is actually not necessary because we can reason that the SIR simulation *will always* reach an equilibrium in finite steps thus not requiring an actual time-limit - we discuss this more in-depth in Appendix B.

10.2.1 Random Event Sampling

An interesting question is whether or not these properties depend on correct interdependencies of events the agents send to each other in reaction to events they receive. Put in other words: do these invariants also hold under *random event sampling*? To test this, instead of using the actual SIR implementation, which inserts the events generated by the agents into the event-queue, we wrote a new SIR kernel. It completely ignores the events generated by the agents and instead makes use of an infinite stream of random queue-elements from which it executes a given number, 100,000 in our case. Note that queue-elements contain a time-stamp, the receiver agent id and the actual event: the time-stamp is ensured to be increasing, to hold up the monotonic time property, the receiver agent id is drawn randomly from the constant list of all agents in the simulation and the actual event is generated completely randomly. As it turns out, the implementation of the agents ensure that the SIR properties are also invariant under *random event sampling* - all tests pass.

10.3 Time-driven

We can expect that the invariants above also hold for the time-driven implementation. The property-test is exactly the same, with the time-driven implementation running instead of the even-driven one. A big difference is that is not necessary to check the property of monotonic increasing time, as it is an invariant statically guaranteed by arrowized FRP through the Yampa implementation. Due to the fact that the flow of time is always implicitly forward and no time-variable is explicitly made accessible within the code, it is not possible to violate the forward flow of time. Because of this, there is no need to check this property explicitly.

When we run the property-test we get a big surprise though: after a few test-cases the property-test fails due to a violation of the invariants! After a little bit of investigation it becomes clear that the invariant *(3) number of susceptible agents is monotonic decreasing* is violated: in the failing test-case the number of susceptible agents is monotonic decreasing with the exception of one step where it *increases* by 1 just to decrease by 1 in the next step. A coverage test reveals that this happens in about 66% of 1,000 test-cases.

The technicalities of the problem are highly involved and not provided in depth here. The source of the problem are the semantics of *switch* and *dpSwitch* which could lead to a delayed output of the agent-state, leading to inconsistencies when feeding it back as environment in the next step. The solution is to delay the output of the susceptible agent by one step using *iPre* as already shown in the original time-driven implementation of 4.1. This solves the problem and the property-test passes.

10.4 Comparing time- and event-driven

Having two conceptually different implementations of the same model, an obvious questions we want to answer is whether they are producing the same dynamics or not. To be more precise, we need to answer the question whether both simulations produce the same distributions under random model parameters and simulation time. This is a perfect use-case for QuickCheck as well and easily encoded into a property-test.

We generate random values for β (contact rate), γ (infectivity) and δ (illness duration) as well as a random population and a random duration to run the simulations for. Note that we restrict γ to be drawn from the (0,1) range as it represents a probability; the random duration is drawn from the (0, 50) range to reduce the run-time duration to a reasonable amount without taking away the randomness.

Both simulation types are run with the same random parameters for 100 replications, collecting the output of the final step. The samples of these replications are then compared using a Mann-Whitney test with a 95% confidence (p-value of 0.05). The reason for choosing this statistical test over a two sample T-Test is that the Mann-Whitney test does not require the samples to be

normally distributed. We know both from experimental observations and discussions in [101] that both implementations produce a bimodal distribution, thus we have to use a non-parametric test like Mann-Whitney to compare them. We further discuss the issue of bimodality in Chapter 11.

We expect a high coverage of at least 90%, which makes our assumption explicit that we expect both simulations to produce highly similar distributions despite their different underlying implementations.

```
prop_event_time_equal :: Positive Int    -- ^ beta, contact rate
                      -> Probability     -- ^ gamma, infectivity, within (0,1) range
                      -> Positive Double -- ^ delta, illness duration
                      -> TimeRange       -- ^ time to run within (0, 50) range
                      -> [SIRState]      -- ^ population
                      -> Property
prop_event_time_equal
    (Positive cor) (P inf) (Positive ild) (T t) as = checkCoverage (do
  -- run 100 replications for time- and event-driven simulation
  (ssTime, isTime, rsTime)    <- unzip3 <$> genTimeSIRRepls 100 as cor inf ild t
  (ssEvent, isEvent, rsEvent) <- unzip3 <$> genEventSIRRepls 100 as cor inf ild t

  -- confidence of 95 for Mann Whitney test
  let p = 0.05
  -- perform statistical tests
  let ssTest = mannWhitneyTwoSample ssTime ssEvent p
      isTest = mannWhitneyTwoSample isTime isEvent p
      rsTest = mannWhitneyTwoSample rsTime rsEvent p

  let allPass = ssTest && isTest && rsTest

  -- add the test to the coverage tests only if it passes.
  return
    (cover 90 allPass "SIR implementations produce equal distributions" True)
```

Indeed when running this test, enforcing QuickCheck to perform sequential statistical hypothesis testing with *checkCoverage*, after 800 tests QuickCheck passes the test.

```
+++ OK, passed 800 tests
    (90.4% SIR event- and time-driven produce equal distributions).
```

This result shows that both implementations produce highly similar distributions although they are not exactly the same as the 10% of failure shows. We will discuss this issue in a broader context in Chapter Chapter 11.

10.5 Discussion

In this chapter we have shown how to encode properties about simulation dynamics, generated by executing agents over time. This allowed to encode actual laws of the underlying SIR model in code and check them under random model parameters.

In the case of the time-driven implementation we saw that our initial assumption, that the invariants will hold for this implementation as well was wrong: QuickCheck revealed a *very* subtle bug in our implementation. Although the probability of this bug is very low, QuickCheck found it due to its random testing nature. This is another *strong* evidence, that random property-based testing is an *excellent* approach for testing Agent-Based Simulations. On the other hand, this bug revealed the difficulties in getting the subtle semantics of FRP right to implement pure functional ABS. This is a strong case that in general an event-driven approach should be preferred, which is also much faster and also not subject to the sampling issues discussed in Chapter 4.1.

Finally we showed that property-based testing also allows to compare two conceptually different implementations of the same underlying model with each other. This is indeed a perfect use-case for property-based testing as it compares whole distributions and not only single runs using unit tests, making this another strong case for the use of property-based testing in ABS.

Chapter 11

Testing the SIR model specification

In the previous chapters we have established the correctness of our event- and time-driven implementation up to our informal specification, we derived from the formal SD specification from Chapter 2.2.1. What we are lacking is a verification whether the implementations also match the formal SD specification or not. In the process of verification, we need to make sure it is correct up to some specification. We aim at connecting the agent-based implementation to the SD specification, by formalising it into properties within a property-test. The SD specification can be given through the differential equations shown in Chapter 2.2.1, which we repeat here:

$$\begin{aligned} \frac{\mathrm{d}S}{\mathrm{d}t} &= -infectionRate & infectionRate &= \frac{I\beta S\gamma}{N} \\ \frac{\mathrm{d}I}{\mathrm{d}t} &= infectionRate - recoveryRate & recoveryRate &= \frac{I}{\delta} \\ \frac{\mathrm{d}R}{\mathrm{d}t} &= recoveryRate \end{aligned} \tag{11.1}$$

Solving these equations is done by integrating over time. In the SD terminology, the integrals are called *Stocks* and the values over which is integrated over time are called *Flows*. At $t = 0$ a single agent is infected because if there wouldn't be any infected agents, the system would immediately reach equilibrium - this is also the formal definition of the steady state of the system: as soon as $I(t) = 0$ the system won't change any more.

$$S(t) = N - I(0) + \int_0^t -infectionRate\,\mathrm{d}t \tag{11.2}$$

$$I(0) = 1 \tag{11.3}$$

$$I(t) = \int_0^t infectionRate - recoveryRate\,\mathrm{d}t \tag{11.4}$$

$$R(t) = \int_0^t recoveryRate\,\mathrm{d}t \tag{11.5}$$

11.1 Deriving a property

The goal is now to derive a property which connects those equations with our implementation. We have to be careful and realise a fundamental difference between the SD and ABS implementations: SD is deterministic and continuous, ABS is stochastic and discrete. Thus we cannot compare single runs but we can only compare averages: stated informally, the property we want to implement is that the ABS dynamics matches the SD ones *on average*, independent of the finite population size, model parameters β (contact rate), γ (infectivity) and δ (illness duration) and duration of the simulation. To be able to compare averages, we run 100 replications of the ABS simulation with same parameters except a different random-number generator in each replication and collect the output of the final steps. We then run a two-sided T-Test on the replication values with the expected values from an SD simulation.

```
compareSDToABS :: Int      -- ^ Initial number of susceptibles
               -> Int      -- ^ Initial number of infected
               -> Int      -- ^ Initial number of recovered
               -> [Int]    -- ^ Final number of susceptibles in replications
               -> [Int]    -- ^ Final number of infected in replications
               -> [Int]    -- ^ Final number of recovered in replications
               -> Int      -- ^ beta (contact rate)
               -> Double   -- ^ gamma (infectivity)
               -> Double   -- ^ delta (illness duration)
               -> Time     -- ^ duration of simulation
               -> Bool
compareSDToABS s0 r0 i0
               ss is rs
               beta gamma delta t = sTest && iTest && rTest
  where
    -- run SD simulation to get expected averages
    (s, i, r) = simulateSD s0 i0 r0 beta gamma delta t

    confidence = 0.95
    sTest = tTestSamples TwoTail s (1 - confidence) ss
    iTest = tTestSamples TwoTail i (1 - confidence) is
    rTest = tTestSamples TwoTail r (1 - confidence) rs
```

The implementation of *simulateSD* is discussed in-depth in Appendix A. We are very well aware that comparing the output against an SD simulation is

dangerous: after all, why should be trust the SD implementation? As outlined in the Appendix A, great care has been taken to ensure the correctness: the formulas from the SIR specification are directly encoded in code, allowed by Yampas arrowized FRP which guarantees that at least that translation step is correct - we then only rely on a small enough sampling rate and the correctness of the Yampa library. The former one is very well in our reach and we pick a sufficiently small samply rate; the latter one is beyond our reach but we expect the library to me mature enough to be correct for our purposes.

11.2 Implementing the test

Implementing a property-test is straight-forward. Here we give the implementation for the time-driven SIR implementation, the implementation for the event-driven SIR implementation is exactly the same with the exception of *genTimeSIRRepls*. We again make use of the *checkCoverage* feature of QuickCheck to get statistical robust results and expect that in 75% of all test-cases the SD and ABS dynamics match *on average* - we discuss below why we chose to use a 75% coverage. QuickCheck will run as many tests as necessary to reach a statistically robust result which either allows to reject or accept this hypothesis.

```
prop_sir_time_spec :: Positive Int     -- ^ beta, contact rate
                   -> Propability      -- ^ gamma, infectivity, within (0,1) range
                   -> Positive Double  -- ^ delta, illness duration
                   -> TimeRange        -- ^ time to run within (0, 50) range
                   -> [SIRState]       -- ^ population
                   -> Property
prop_sir_time_spec
    (Positive cor) (P inf) (Positive ild) (T t) as = checkCoverage (do
  -- get initial agent numbers
  let (s0,i0,r0) = aggregateSIRStates as
  -- run 100 replications of time-driven SIR implementation
  (ss, is, rs) <- unzip3 <$> genTimeSIRRepls 100 as cor inf ild t
  let prop = compareSDToABS s0 i0 r0 ss is rs cor inf ild t
  return $ cover 75 prop "SIR time-driven passes t-test with simulated SD" True
```

11.3 Running the test

When running the tests for the time- and event-driven implementation, QuickCheck reports the following:

```
+++ OK, passed 400 tests
    (85.2% SIR time-driven passes t-test with simulated SD).

+++ OK, passed 3200 tests
    (74.84% SIR event-driven passes t-test with simulated SD).
```

The results clearly show that in both cases we reach the expected 75% of coverage: the distributions of the time- and event-driven implementations match

the simulated SD dynamics to at least 75%, in case of time-driven this is even substantially higher. Still, this result raises a few questions:

1. Why does the performance of the time-driven implementation surpasses the event-driven one by more than 10%?

2. Why are we not reaching a far higher coverage beyond 90% and why have we chosen 75% in the first place? After all our initial assumption was that the time- and event-driven implementations are simply agent-based implementations of the SD model and thus their dynamics should generate the same distributions as the SD ones.

First of all, the results are a very strong indication that although both implementation techniques try to implement the same underlying model, they generate different distributions and are thus not *statistically* equal. This was already established in Chapter 10, where we have compared the distributions of both simulations and found that although we reach 90% similarity this means that they are still different in some cases. The results of this property-test reflect that as well and we argue that this is also the reason why we see different performance of each when compared to SD.

An explanation why the time-driven approach seems to be closer to the SD dynamics is that in the event-driven approach we are dealing with discrete events, jumping from time to time instead of moving forward in time continuously as it happens conceptually in the time-driven approach. Time is also continuous in SD, thus it seems intuitively clear that a time-driven approach is closer to the SD implementation than the event-driven one - it seems valid to call our time-driven approach a continuous agent-based simulation approach. The implication is that depending on our intention, picking a time-driven or an event-driven implementation can and will make a statistical difference. If one is transferring an SD to an ABS model, one might consider to follow the time-driven approach as it seems to come much closer to the SD dynamics than the event-driven approach.

The reason that we are not reaching a coverage level up to and beyond 90% is rooted in the fundamental difference between SD and ABS: due to ABS' stochastic nature, its dynamics cannot match an SD exactly because it generates a *distribution* whereas the SD is deterministic. This enables ABS to explore and reveal paths which are not possible in deterministic SD. In the case of the SIR model, such an alternative path would be the immediate recovery of the single infected agent at the beginning without infecting any other agent. This is not possible in the SD case: in case there is 1 infected agent, the whole epidemic will unfold.

The difficulty of comparing dynamics between SD and ABS and the impracticality to compare them *exactly* was shown by [101] in the case of the SIR model, where the authors showed that it generates a bimodal distribution. Further, the authors report that a 70% envelope contains both the results of the SD and ABS implementation which is the reason why we chose a a 75% coverage as

our initial guess, which has turned out to work well and is in accordance with the results of [101].

The question which remains is whether it actually even makes sense to compare the approaches to SD or even amongst each other - after all they can be seen as fundamentally different approaches. We can argue that they are qualitatively equal as [53] has already emphasised in a different study on comparing ABS and SD: although dynamics of ABS models are statistically different from SD ones, they look similar. The main difference is that ABS can contribute additional insight through revealing extra patterns due to its stochasticity, something not possible with SD. Thus in the end we simply have to accept that the respective coverage ratios are the closest we can get and that this is also the closest we can get in terms of validating our implementations against the original SD specification.

11.4 Discussion

After having shown in previous chapters, that individual agent behaviour is correct up to some specification, in this chapter we focused on validating the dynamics of the simulation with the original SD specification.

By using QuickCheck, we showed how to connect both ABS implementations to the SD specification by deriving a property, based on the SD specification. This property is directly expressed in code and tested through generating random test-cases with random agent populations and random model parameters.

Although our initial idea of matching the ABS implementation to the SD specifications has not worked out in an exact way, we still showed a way of formalizing and expressing these relations in code and testing them using QuickCheck. The results showed that the ABS implementation comes close to the original SD specification but does not match it exactly - it is indeed richer in its dynamics as [101, 53] have already shown. Our approach might work out better for a different model, which has a better behaved underlying specification than the bimodal SIR.

In this part of the thesis we had an extensive look into the usefulness of randomised property-based testing in the development, specification and testing of pure functional ABS. We found property-based testing particularly well suited for ABS firstly due to ABS stochastic nature and second because we can formulate specifications, meaning we describe *what* to test instead of *how* to test. Also the deductive nature of falsification in property-based testing suits very well the constructive and often exploratory nature of ABS.

Indeed, we can see property-based testing not only as a post-implementation testing tool but as an extension to the development process where the developer engages in an interactive cycle of implementing agent and simulation behaviour and then immediately putting specifications into property-tests and running them. This approach of expressing specifications instead of special cases like in unit tests is arguably a much more natural approach to test-driven development in ABS development than only relying on unit tests.

In this part we only focused on the explanatory SIR model and ignored the exploratory Sugarcape. It is important to understand that testing of exploratory models is also possible through hypothesis testing. We discuss this approach in Appendix C in the context of validating our Sugarscape implementation.

We have only touched the tip of the iceberg and expect tremendous potential from applying property-based testing to different kind of models and in implementing ABS in general. Indeed, although property-based testing has its origins in Haskell, similar libraries have been developed for other languages e.g. Java, Pyhton, C++ as well and we hope that our research has sparked an interest in applying property-based testing to the established object-oriented languages in ABS as well.

Part V:

Discussion and Conclusion

In this part an in-depth, highly critical evaluation of the aim, objective and hypotheses of the introduction follows, which puts the techniques and contributions of this thesis into perspective. This part finishes with a brief conclusion to the thesis were also further research is discussed.

Chapter 12

Discussion

This thesis started out by challenging the established views that *"[..] object-oriented programming to be a particularly natural development environment for Sugarscape specifically and artificial societies generally [..]"* [49] (p. 179) and that *agents map naturally to objects* [113]. As a highly challenging alternative, a radical different approach to implementing ABS was proposed, using the pure functional programming paradigm. The language of choice Haskell was motivated due to its matureness, increasing relevance to real-world applications and leading in pure functional programming concepts.

The conjecture was that by using Haskell, one can directly transfer the promises made by pure functional programming to ABS as well, directly gaining a few highly important benefits:

1. The static strong type system allows to remove a substantial number and classes of bugs at run-time and if one programs careful one can even guarantee that no bugs as in crashes or exceptions will occur at run-time. This is especially true for purely computational problems (without IO) as ABS almost always are.

2. Explicit handling and control of side-effects delivers even more static guarantees at compile time and allows to deal with deterministic side-effects (random-number streams, read-/write only contexts, state) in a referential transparent way. In combination with strong static typing this allows to reduce logical bugs (subject to the domain of the problem) by dramatically reducing available and valid operations on data - after all stateful applications are a fact, the challenge is how to deal with state. As ABS is full of state due to agents and the environment, this seems to be an obvious great thing to have to increase correctness of an implementation. Further, this should allow to produce an implementation which is guaranteed to reproducible (runs with same initial conditions *will* result in same dynamics) at compile time.

3. Parallel and concurrent programming is seen to be lot easier, less painful

and less error prone in functional programming in general and in Haskell in particular due to immutable data and the explicit side-effects. The concept of Software Transactional Memory, which offers to formulate a problem as a data-flow problem like there was no concurrency seemed highly promising. Besides, data-parallel programming promises to speed up code without the need for changing any of the logic or types. This seemed to offer a straightforward way of speeding up ABS implementations either through data-parallelism or concurrency. This has always been quite difficult to achieve in traditional ABS due to OO and pure functional programming seems to offer a solution.

4. The data-centric declarative style, referential transparency and immutability of data makes testing substantially easier due to composability: functions can be easily tested in isolation from each other even if they involve side-effects. This opens the door for (randomised) property-based testing which intuitively seemed to be a perfect match to test ABS implementations which are (almost) always stochastic in nature.

The relevance of each of these promises to ABS is pointed out in the respective promise and it is quite obvious that these benefits would clearly be of immense value in ABS, with the common baseline that they all support implementations of ABS to be more likely to be correct - something of fundamental value in simulation. At this point we argue that the thesis was able to successfully show that all promises transfer to ABS implementations and we give a holistic reflection and critique of them in the subsequent sections.

12.1 How

TODO ARGUMENT - missing OO definition

The central question which needed to be answered first was *how* ABS could be done pure functionally, as there didn't exist any research which offered a systematic solution to that problem. More specifically, it was unclear how to represent agents, how to express agent identity, local agents state, changing behaviour and interactions amongst agents and the environment. After all, this is straightforward in OO due to mutable shared state encapsulated in objects.

The solution was to use arrowized FRP both in the pure implementation of Yampa and the monadic version as in the library Dunai. Building on top of them allowed us to implement pro-activity of agents, encapsulation of local agent state, an environment as shared mutable state and synchronous agent-interactions based on an event-driven approach. The central concept behind these approaches are Signal Functions (SF), generalised in Dunai to Monadic Stream Functions (MSF), which are implemented using closures and continuations, fundamental building blocks and concepts of pure functional programming.

SF and MSF can be seen as very simple *immutable* objects with a single method following a *shared nothing* semantics as mentioned in Chapter 6 already.

This interpretation and the fact that we seem to achieve encapsulation of local agent state and interactions obviously raises the question if agents actually *do* map naturally to objects - after all, despite being in a pure functional setting, we are talking about objects again!

It seems that we indeed have to agree that agents do actually map naturally to objects. However, throughout the course of this thesis it became clear that we have to think objects in a much broader context than the one of existing OO terminology as in the popular family of Java, C++ and Python. The reason that we have shown that we can represent agents as objects also in a purely functional way, leads us to the question, what actually constitutes objects and we have to be careful not to confuse the *concept* of objects with their *implementation* within a language.

There does not exist a commonly agreed upon definition of objects and OO but rather a bunch of ideas and concepts [1]. It is agreed that the original ideas of objects and OO were conceived by Kristen Nygaard, the inventor of Simula 67, the first object-oriented language [39] and Alan Kay, the inventor of SmallTalk, another pioneering object-oriented language in the early 70s [92].

Kristen Nygaard identified object-oriented programming by *"A program execution is regarded as a physical model, simulating the behaviour of either a real or imaginary part of the world."*, thus he puts the focus on the modelling aspect of the problem. Alan Kay claims to have coined the term *object-oriented* and defines it in more technical terms: everything is an object; every object is an instance of a class; the class holds the shared behaviour for its instances; objects communicate by sending and receiving messages. Alan Kay puts a strong emphasis on sending and receiving messages, with a shared-nothing interpretation. This becomes especially clear in a quote attributed to him: *"The big idea is "messaging" ... "I invented the term Object-Oriented and I can tell you I did not have C++ in mind."*.

So we see that the original *concepts* of objects and OO vary considerably from how objects and OO is *implemented* today in the family of popular OO languages like Java, C++ and Python. The most substantial different to the original definition of Kay is that messages are not pure data - they do not follow a shared nothing semantics. This leads to the failure of objects to compose behaviour and encapsulate data properly [18], [50]. Ironically, this has always been the main argument for advertising the use of object oriented programming. The reason for this is that objects hide both *mutation* and *sharing through pointers or references* of object-internal data. This makes data-flow mostly implicit due to the side-effects on the mutable data which is globally scattered across objects. To deal with the problem of composability and implicit data-flow the seminal work [59] put forward the use of *patterns* to organize objects and their interaction. Other concepts, trying to address the problems, were the SOLID principles and Dependency Injection.

Despite these advances in understanding the OO paradigm and how to use

[1] `http://wiki.c2.com/?DefinitionsForOo`

it properly, the increased complexity leads to an inherent difficulty to express and follow data-flow in an OO program and exploit parallelism and concurrency due to mutable shared state. Even worse, concurrency breaks encapsulation of objects as well and prevents composing them.

The rise of functional concepts in OO languages in the last years are a strong indication that OO is lacking features which have existed in FP for decades. Java 8 added lambda expressions and functional style programming using map, fold, reduce, filter, which together with lambdas allow a data-flow oriented approach to computing. Python, which surges in popularity within the OO family of languages, allows very data-flow centric and functional style of programming through lambda functions, list comprehensions and other functional features as it does not require programmers to stick to the OO paradigm. Popularisation of JavaScript frameworks like React, Elm and Purescript, which emphasise a functional, data-flow driven approach of web-programming. Thus it seems that functional concepts overcome the weakness of OO to model explicit, immutable data-flows which can be exploited towards easier parallelisation and concurrency.

All these properties of explicit data-flow and applicability of parallelism and concurrency are highly desirable when implementing Simulations: it is a fact that simulations are data-centric, that is they are all about about consuming, processing and producing data and they have to do it fast and correct. ABS being simulation methodology is no exception to that fact.

The question is then why not use toolkits like Matlab or R - after all they are completely data-centric? This would be the other extreme, just like OO is and we would run into difficulties as well. The point is that ABS is not purely data-centric either and is indeed richer: agents can interact with each other and with an environment. So we have a tension here: ABS is data-centric on the one hand, and interaction-centric on the other - can we combine both worlds? Our approach is *one* answer to do that in a pure, strong statically typed language - Haskell. It can be seen as an object-centric approach, which *implements* a very simple *concept* of shared-nothing, immutable, pure functional objects.

12.2 Benefits

After having established *how* to do pure functional ABS in a robust and maintainable way the question was: does our approach leverage and deliver the promises of functional programming as well: what are its benefits? We have discussed them in the respective chapters already at length and will thus only recap them here in a broader context.

12.2.1 Static guarantees

Probably the biggest strength is that we can guarantee reproducibility at compile time: given identical initial conditions, repeated runs of the simulation will lead to same outputs. This is of fundamental importance in simulation and addressed in the Sugarscape model: *"... when the sequence of random numbers*

is specified ex ante the model is deterministic. Stated yet another way, model output is invariant from run to run when all aspects of the model are kept constant including the stream of random numbers." (page 28, footnote 16) - we can guarantee that in our pure functional approach already *at compile time*.

Further, we can enforce update semantics to a certain degree by dramatically restricting the operations on state and the available state to agents. For example, in the time-driven approach the fact that the environment is provided as read-only and agents cannot interfere with other agents due to purity and complete lack of side-effects, factually enforces the parallel update strategy: there is simply no way for agents to misbheave and violate semantics of updates by mutating state they are not allowed to.

Another fundamental strength is the power of polymorphism in Haskell, which goes far beyond the polymorphism [2] of existing object oriented languages. We see a particular instance of that in the polymorphism we developed in the concepts behind Sugarscape: we can compose effects depending on the model and we can easily swap out environment and events with very few changes with the benefit that the compiler will inform us about breaking changes. This is directly related to refactoring, which is very convenient and quickly becomes the norm in the development process: guided by types (change / refine them) and relying on the compiler to point out problems, results in very effective and quick changes without danger of bugs showing up at run-time. This is not possible in dynamicall OO languages like Python because of its lack of compiler and types, and much less effective in Java due to its dynamic type-system which is only remedied through strong IDE support.

Note that this thesis directly capitalises on the fact that most ABS models are primarily of computational nature, thus CPU bound and do not involve IO *inside the agents* while running the simulation. The concurrent approach with STM is an exception but at least we retain the guarantees that the nondeterminism within the agent behaviour originates from the concurrency using STM and nothing else. Even if some IO is required, like rendering the simulation as we did in Sugarscape, due to the lose coupling and compositional qualities of pure functional programming it is straightforward to separate these concerns and keep the impure rendering parts from the pure agent behaviour. If there arises the use-case where agents absolutely need to perform some impure IO within their behaviour then there exist two options. The first one is to let agents construct IO actions and pass them to the simulation kernel for execution, requiring the simulation kernel to run now in IO instead of being pure. This is especially suitable for one-way IO actions, where an agent does not need to synchronously wait for a result. If a synchronous IO action is required with the agent waiting for a result, it could be communicated back from the simulation kernel. This keeps the agent behaviour still pure but with the consequence of indirection and higher complexity. The other option is to simply run agents within the IO Monad - then everything is possible and all bets are off regarding static guarantees and reproducibility.

[2] Yes, polymorphism is not unique to OO

12.2.2 Parallelism and Concurrency

Adding data-parallelism is easy and often requires simply swapping out a data-structure or library function against its parallel version. Concurrency, although still hard, is less painful to address and add in a pure functional setting due to immutable data and explicit side-effects. Further, the benefits of implementing concurrent ABS based on Software Transactional Memory (STM) has been shown at length in the respective part which underlines the strength of Haskell for concurrent ABS due to its strong guarantees about retry-semantics.

12.2.3 Property-Based Testing

Testing in general allows much more control and checking of invariants due to the explicit handling of effects - together with the strong static type system, the testing-code is in full, explicit control over the functionality it tests. Property-based testing in particular is a perfect match to testing ABS due to the random nature in both and because it supports convenient expressing of specifications. Thus we can conclude that in a pure functional setting, testing is very expressive and powerful and supports working towards an implementation which is very likely to be correct. For further insight into testing Functional Reactive Programs we can directly leverage on the work of [123]. A classic use-case which is a unique benefit of pure functional programming, namely *equational reasoning* was not investigated in this thesis as it was beyond the focus of this Ph.D. We expect that this technique is applicable to parts of our approach as well but leave this for further research.

12.3 Drawbacks

Obviously nothing comes without drawbacks, and also our approach suffers from a few. We discuss them here and propose solutions where applicable.

12.3.1 Efficiency

Currently, the performance our approaches does not come close to imperative implementations, as shown in the discussions of each respective chapters. There are two main reasons for it: first, FP is known for being slower due to higher level of abstractions, which are bought by slower code in general and second, updates are the main bottleneck due to immutable data requiring to copy the whole (or subparts) of a data structure in cases of a change. The first one is easily addressable through the use of data-parallelism and concurrency as shown in Chapter 7 and 8. The second reason can be addressed by the use of linear types [16], which allow to annotate a variable with how often it is used within a function. From this a compiler can derive aggressive optimisations, resulting in imperative-style performance but retaining the declarative nature of the code. Also the use of monad transformer stacks has performance implications which can be quite subtle but can be alleviated by careful usage and re-ordering of

lifts which might result in increased performance e.g. instead of mapM (lift ...) do lift (mapM ...).

However, it was shown by various people [142, 143, 96] that it is possible to reach C speed in Haskell as well. The direction to do this is using the worker/wrapper transformation [60], clever combination of techniques with strict *foldl'* and data-declaration with strictness annotation instead of lazy tuples and Stream Fusion [38, 104]. The problem is of course that to apply these techniques one needs to have deep knowledge of Haskell and its subtle details of (lazy) evaluation, making this a very non-trivial task. A problem is that those techniques seem only applicable in a context of a tight loop which crunches numbers of a list, thus it is not directly applicable in our case as we are clearly bound by the effectful computations: MSF and Monad Transformers are the limiting factor, not inner loops.

Concluding we can say that the current performance makes our approach not very attractive for real-world use *at the moment*. Also the fact that the sequential OO implementation seems to outperform the concurrent and parallel implementations as well, seems to question our motivation as why to use pure functional programming and parallel computation at all. Still, the bad performance results do not invalidate our research as this thesis aim is not the development of high-performance pure functional implementations but rather exploring concepts of ABS in pure functional programming which are only first steps and need to be developed further into something to be used in the real world. We don't think that our pure functional approach will be able to reach the Java performance but we think that it should be possible to come considerably closer, making it more applicable for real-world usage. We leave a deeper investigation of this problem for further research.

12.3.2 Space-Leaks

Haskell is notorious for its memory-leaks due to lazy evaluation: data is only evaluated when required. Even for simple programs one can be hit hard by a serious space-leak where unevaluated code pieces (thunks) build up in memory until they are needed, leading to dramatically increased memory usage. It is no surprise that our highly complex Sugarscape implementation initially suffered severely from space-leaks, piling up about 40 MByte / second. In simulation this is a big issue, threatening the value of the whole implementation despite its other benefits: because simulations might run for a (very) long time or conceptually forever, one must make absolutely sure that the memory usage stays somewhat constant. As a remedy, Haskell allows to add so-called strictness pragmas to code-modules which forces strict evaluation of all data even if it is not used. Carefully adding this conservatively file-by file applying other techniques of forcing evaluation removed most of the memory leaks.

Another memory leak was caused by selecting the wrong data-structure for our environment, for which we initially used an immutable array. The problem is that in the case of an update the whole array is copied, causing memory leaks AND a performance problem. We replaced it by an IntMap which uses

integers as key (mapping 2d coordinates to unique integers is trivial) and is internally implemented as a radix-tree which allows for very fast lookups and inserts because whole sub-trees can be re-used.

12.3.3 Productivity and learning curve

A case study in [69] hints that simply by switching to a static type system alone does not gain anything and can even be detriment. It also needs to have a certain level of abstractions like Haskell type system does or even dependent types as in Idris. Although such case-studies have to be taken with care, there is also some truth in it: working in a statically strong type system prevents the developer from moving quickly and making quick and dirty changes. This can be both a benefit and a drawback: in general it prevents from breaking changes which show only up at compile time as in dynamic languages but at the same time the whole program is much more rigid and a proper structure needs to be thought out and designed often up-front, slowing down the process. However, this is a contribution of this thesis that it outlines exactly these structures within ABS so that implementers who want to use the same approach do not have to reinvent the wheel.

A more severe problem is that pure functional programming, especially Haskell is seen as hard to learn with a steep learning curve. This and the fact that pure functional ABS achieves similar things as existing OO approaches puts a high barrier to implementers picking up a pure functional approach to ABS. Thus the lack of availability of Haskell expertise can be enough to pose a serious drawback even if the approach of this thesis seem to be desirable in a project.

12.3.4 Agent interactions

This thesis is *one* way of showing how to separate both and reap the benefits. A time-driven ABS like SIR or an ACE with simple agents not interaction with each other like ZI traders is heavily data-centric and very low on agent-interaction. Such data-driven ABS models are quite well expressed in a purely functional approach with the advantage that one can reap the benefits of reproducibility at compile time, using STM for concurrency and property-based testing for verification and validation. An event-driven simulation with complex agent state and agent-interactions like social simulations like Sugarscape or Chemical or Biology simulation with cell interactions are also possible in a pure functional setting as we have shown in the case of the Sugarscape model. Although we were able to give a good solution to complex agent state and synchronous, direct Agent-interactions in our event-driven SIR and Sugarscape and they *do* work in Haskell, they are cumbersome to get right without library support and as we pointed out in the STM chapter, it seems that this approach to synchronous bi-directional agent-interactions is not applicable to concurrency with STM.

This has lead to the fundamental conclusion of this thesis, that although we have shown the benefit of functional programming in ABS, in models which require complex agent-interactions in a potentially concurrent we are hitting the limits of the pure functional approach here. The reason for it is that ultimately although agents do map naturally to objects they are even more naturally represented using actors.

The Actor-Model, a model of concurrency, was initially conceived by Hewitt in 1973 [76] and refined later on [74], [75]. It was a major influence in designing the concept of agents and although there are important differences between actors and agents there are huge similarities thus the idea to use actors to build agent-based simulations comes quite natural. The theory was put on firm semantic grounds first through Irene Greif by defining its operational semantics [66] and then Will Clinger by defining denotational semantics [34]. In the seminal work of Agha [1] he developed a semantic mode, he termed *actors* which was then developed further [2] into an actor language with operational semantics which made connections to process calculi and functional programming languages (see both below).

An actor is a uniquely addressable entity which can do the following *in response to a message*

- Send an arbitrary number (even infinite) of messages to other actors.
- Create an arbitrary number of actors.
- Define its own behaviour upon reception of the next message.

In the actor model theory there is no restriction on the order of the above actions and so an actor can do all the things above in parallel and concurrently at the same time. This property and that actors are reactive and not pro-active is the fundamental difference between actors and agents, so an agent is *not* an actor but conceptually nearly identical and definitely much closer to an agent in comparison to an object. The actor model can be seen as quite influential to the development of the concept of agents in ABS, which borrowed it from Multi Agent Systems [166]. Technically, it emphasises message-passing concurrency with share-nothing semantics (no shared state between agents), which maps nicely to functional programming concepts.

The programming-model of actors [1] was the inspiration for the Erlang programming language [6], which was created in the 1980's by Joe Armstrong for Eriksson for developing distributed high reliability software in telecommunications. The implication is that, the focus would shift immediately to the use of the actor model for concurrent interaction of agents through messages. The languages type-system is strong and dynamic and thus lacks type-checking at compile-time. Thus the structure of computation plays naturally no role because we cannot look at it from the abstract perspective as we can in Haskell. Purity can not be guaranteed and due to agents being processes concurrency is everywhere, and even though it is very tamed through shared-nothing messaging semantics, this implies that repeated runs with same initial conditions

might lead to different results. Obviously we could avoid implementing agents as processes but then we basically sacrifice the very heart and feature of the language.

Despite its focus on messages, Erlang is a functional languages, which puts you into the data-centric approach: messages are pure data with *shared nothing semantics*. This makes testing easier and also opens the way for property-based testing which is available in Erlang as well where it even allows to detect race conditions [33].

We hypothesize that an true concurrent actor approach like Erlang is substantially more natural, much more performant and opens up for concurrency. its main drawback is its dynamic type system which reduces guarantees we have about correctness at run-time, also concurrency leads to different dynamics. We have prototyped highly promising concurrent event-driven SIR and Sugarscape implementations in Erlang and they supports our hypothesis. Unfortunately, an in-depth discussion is beyond the scope of this thesis and which we leave this for highly promising further research in the conclusion.

12.4 The Gintis Case revisited

After having established all the benefits and drawbacks pure functional programming has to offer for ABS, we want to return to the Introduction again, where we mentioned the work of Gintis [62]. To repeat, in this paper Gintis has claimed to have found a mechanism in bilateral decentralized exchange, which resulted in Walrasian General Equilibrium without the neo-classical approach of a tatonement process through a central auctioneer. Due to its high-impact result for economics, researchers [86] tried to reproduce the results independently but were not able to do so. After Gintis provided the code, it was found that there was a bug in his implementation which led to the unexpected results, which were seriously damaged through this error. The work of [51] investigated the specific nature of Gintis bugs and reported the following (Section *3.1.1 Deviations from the paper*, page 23):

1. An agent calculates the optimum inventory (or demand) according to a specific formula, which involves a factor λ which gets computed as $\lambda = \frac{\sum_j p_{ij} x_{ij}}{\sum_j p_{ij} x_{ij}}$. What the specific computation denotes is not important here, what is important is that this computation is always 1. The authors [51] claim that the correct formula should have been: $\lambda = \frac{\sum_j p_{ij} x_{ij}}{\sum_j p_{ij} o_j}$ with o in the denominator instead of x.

2. There seems to be a discrepancy between the paper and the implementation describing the trading of agents. According to the paper the amount they exchange follows $x_{ig} \equiv \frac{p_{ig} x_{ig}}{p_{ih}}$. In the implementation however, Gintis uses $x_{ig} \equiv \frac{p_{ih} x_{ih}}{p_{ig}}$ but seems to do so inconsistently throughout the his code, leading to wrong calculations.

3. Another bug was due to reversed ordering of events, where agents use old prices vectors due to missing recalculation which only happens in the next step.

4. There are a number of other subtle bugs, which, according to the authors [51] seemed to have no impact on the outcome of the simulation: slight miscalculation of the standard deviation for consumer and producer prices, crashing the program at runtime when dividing the agents unequally between different production goods due to a negative random number which in turn raises an exception in the Delphi Random function.

After having claimed that pure functional programming helps in implementing simulations which are more likely to be correct, the following questions arise:

Do the techniques introduced in this thesis transfer to this problem and model as well? The short answer is, yes they obviously do as Gintis models interacting individual agents which consume and produce and trade with each other. This could be implemented both with our time- and event-driven approach, with a better choice probably being the event-driven one due to agents directly trading with each other. However, for some models, our techniques introduced in Part II are too powerful and a much simpler approach would suffice to implement it. In general too much power should always be avoided (at least in programming and software engineering) because with much power comes much responsibility: more power requires to pay more attention to details and thus there is more potential to make mistakes. Thus we should always look for the technique with minimal power but maximum abstraction, which solves our problem sufficiently. Gintis model is such an example: it resides in a very different domain of ABS, called Agent-Based Computational Economics (ACE).

ACE is a very important field, which picked up ABS in recent years. The field of economics is an immensely vast and complex one with many facets to it, ranging from firms, to financial markets to whole economies of a country [24]. Today its very foundations rest on rational expectations, optimization and the efficient market hypothesis. The idea is that the macroeconomics are explained by the micro foundations [35] defined through behaviour of individual agents. These agents are characterized by rational expectations, optimizing behaviour, having perfect information, equilibrium [54]. This approach to economics has come under heavy criticism in the last years for being not realistic, making impossible assumptions like perfect information, not being able to provide a process under which equilibrium is reached [94] and failing to predict crashes like the sub-prime mortgage crisis despite all the promises - the science of economics is perceived to be detached from reality [54]. ACE is a promise to repair the empirical deficit which (neo-classic) economics seem to exhibit by allowing to make more realistic, empirical assumptions about the agents which form the micro foundations. The ACE agents are characterized by bounded rationality, local information, restricted interactions over networks and out-of-equilibrium

behaviour [52]. Works which investigate ACE as a discipline and discuss its methodology are [147], [130], [14], [19]. Tesfatsion [148] defines ACE as *[...] computational modelling of economic processes (including whole economies) as open-ended dynamic systems of interacting agents.*.

It is important to understand, that ACE utilises ABS different than the social sciences do. The latter one focuses more on agent-interactions, where in ACE the rational and non-rational actions of individual agents are more important. Thus in many ACE models, the full power of the techniques introduced in Part II is not required. More specifically, agents of ACE models tend to have much simpler state, behave often in only one specific way, don't use synchronised agent-interactions and are very rarely located in a spatial environment but focus more on network connections [164, 63] or avoid the notion of connectivity altogether. This is certainly the fact in the case of the Gintis model, as implemented by Gintis himself and the Java implementation of [51]:

- Even though it is an agent-based model and there is a clear notion of agents in the code, where they are represented as objects, the agents are very simple in terms of their structure. They are characterised by a few floating-point values with very simple behaviour that does not change over time.
- There are only very simple direct agent-interactions, exchanging bids and asks, leading to an exchange.
- There is no environment whatsoever and a fully connected network is implicitly assumed because each agent can trade with all other agents.
- The only side-effect necessary in this simulation is to draw random-numbers.

Thus a Haskell implementation in this domain can be achieved completely without the full force of our techniques: agents can be represented as simple data-structures without SFs / MSFs, interactions handled by the kernel, no need for an environment, scheduling is handled directly by the kernel and side-effects are restricted to run in the Random Monad only. Due to the substantial complexity of the Gintis model, we have refrained from attempting a full implementation of it in Haskell. However, to investigate this point more in-depth we implemented a simulation [3] with so called Zero Intelligence traders [64], a well known and fundamental concept found in ACE. Our implementation was inspired by an implementation in Python [4] and is a satisfactory proof-of-concept underlining the fact that we can do ABS also in a robust way without the tremendous power offered by our techniques. However, a full treatment of this is beyond the scope of this thesis and is left for further research.

[3] Available at `https://github.com/thalerjonathan/zerointelligence`

[4] `http://people.brandeis.edu/~blebaron/classes/agentfin/GodeSunder.html`

Would the use of Haskell have prevented the bugs which Gintis made? The first and second bugs as reported above are an indication for a problematic use of indexed lists or arrays. Generally one can say that independent of programming languages, indices into an array or list are *always* problematic because it is very easy to make very subtle mistakes by getting indices wrong. Pure FP would suffer the same problem *if* a similar technique would have been used. However, due to the fact that data in Haskell is immutable, an *idiomatic* implementation, following pure functional programming concepts, we would have probably not seen the use of lists but (Generalised) Algebraic Data Types (GADT), making this kind of bug much less likely. Further, due to the *declarative* nature of pure FP in Haskell, it is more likely that the implementer, reading through the existing code might have spotted the bug: there is much less noise in an idiomatic functional implementation than in imperative code, making code highly expressive and concise, thus less to read and more obvious.

The third bug is a very subtle logical error, regarding the semantics of the simulation. A pure functional alone would not have helped avoiding this mistake. However, we think that due to the declarative nature it would have been possible to spot it, also because data is immutable and the fact that we are dealing with an old version of data is much more explicit.

The last bugs are typical run-time errors, which would and do occur in Haskell as well, so a pure functional approach would not necessarily avoid these kind of bugs. However, such bugs can be avoided by using a dependently typed functional language like Idris [25] as such a type system allow to ensure in the types that only positive random numbers are drawn, and that the input ranges are strictly positive.

Thus summarizing, we hypothesise that with a clean and *idiomatic* pure functional implementation it would have been very likely that Gintis would have avoided or to spot the bugs. Further, we claim that dependent types might have been of substantial benefit in the Gintis case, but we leave this for further research as it is beyond the scope of this thesis (see Appendix B).

Would property-based tests have been of any help to prevent the bugs? We hypothesise that it is very likely that if Gintis would have applied rigorous unit- and property-based testing to his model - which he should have, due to the high impact of his outcome - he would have found the inconsistencies and could have corrected them. The code of [51] contains numerous *checkInvariants* and assertions, which *are* properties expressed in code, thus immediately applicable to property-based testing. Further, due to the mathematical nature of the problem, many properties in the form of formulas can be found in the paper specification, which should be directly expressible using property-based and unit-testing.

12.5 Generalising Research

We hypothesize that our research can be transferred to other related fields as well, which puts our contributions into a much broader perspective, giving it more impact than restricting it just to the very narrow field of ABS. Although the subsequent sections are just conjectures, we argue that our findings might be applicable to the following fields at least on a conceptual level.

12.5.1 Simulation in general

We showed at length in this thesis that purity in a simulation leads to repeatability which is of utmost importance in scientific computation. These insights are easily transferable to simulation software in general and might be of huge benefit there. Also my approach to dependent types in ABS might be applicable to simulations in general due to the correspondence between equilibrium & totality, in use for hypotheses formulation and specifications formulation as pointed out in Appendix B.

12.5.2 System Dynamics

We have implemented a System Dynamics (SD) simulation in Appendix A. Although it is only an implementation of the SIR model, it shows clearly how an SD *specification* can directly be encoded in pure functional programming using arrowised FRP. The approach is simple enough to be generated automatically, is highly performant and could serve as language of choice for an SD simulation engine backend. We leave a deeper exploration of this topic for further research.

12.5.3 Discrete Event Simulation

We have already implemented basic mechanics of a Discrete Event Simulation in the case of the event-driven SIR. Still our approach is quite ABS-centric and it would be very interesting to see whether we can express the DES model network directly in code, guaranteeing compatibility of elements statically at compile time. This should be possible due to the declarative nature of pure functional programming and the process-oriented nature of arrowized Functional Reactive Programming - in the end both DES and FRP model data-flow networks which are fixed at compile time, so it should be a natural fit.

There exists also Parallel DES (PDES) [57], which is concerned about the problems of running a DES in parallel, where the challenge is how to deal with sequential dependencies. Optimistic approaches run them in parallel, just like STM does, and rolls back actions in case sequential orderings are violated. We hypothesize that in a pure functional language with or without STM it should be conceptually easier to implement such rollback semantics due to immutable persistent data-structures and controlled side-effects.

12.5.4 Recursive Simulation

Due to the recursive nature of functional programming we believe that it is also a natural fit to implement recursive simulations as the one discussed in [61]. In recursive ABS agents are able to halt time and anticipate an arbitrary number of actions, compare their outcome to resume time and continue with a specifically chosen action e.g. the best performing or the one in which they haven't died. More precisely, an agent has the ability to run the simulation recursively a number of times where the number is not determined initially but can depend on the outcome of the recursive simulation. So recursive ABS gives each Agent the ability to run the simulation locally from its point of view to project its actions into the future and change them in the present. Due to controlled side-effects and referential transparency, combined with the recursive nature of pure functional programming, we think that implementing a recursive simulation in such a setting should be straight-forward. We leave this for further research.

12.5.5 Multi Agent Systems

The fields of Multi Agent Systems (MAS) and ABS are closely related where ABS has drawn much inspiration from MAS [166], [162]. It is important to understand that MAS and ABS are two different fields where in MAS the focus is more on technical details, implementing a system of interacting intelligent agents within a highly complex environment with the focus on solving AI problems.

Because in both fields, the concept of interacting agents is of fundamental importance, we expect our research also to be applicable in parts to the field of MAS. Especially the work on static guarantees and dependent types should be very useful there because MAS is very interested in correctness, verification and formally reasoning about a system and their agents, to show that a system follows a formal specifications.

12.6 When not

We are very well aware that our approach has yet to reach maturity and prove itself in time in real simulation studies. This fact that it has to prove its value in time, that it is missing a mature and stable library yet (see future research) and the fact that there exist a bunch the industry strength tool kits and libraries (Repast, NetLogo, AnyLogic) and the widespread use and knowledge of OO which makes abs implementers readily available, makes OO still the highly compelling approach to implement ABS. This allows for a quick and cheap implementation of low-impact and straightforward models where the need for correctness, reproducibility, verification and validation is not of primary concern. Also as outlined, performance in FP is still nowhere near OO although that argument might get diminished by the potential of using actor based concurrency like in Erlang to implement ABS. Another benefit is that OO as a modelling tool to a problem is still highly useful in the case of UML.

Chapter 13

Conclusion

This thesis has shown at length *how* pure functional ABS is possible in a robust maintainable way and *why* it is of benefit and when a pure functional approach should be *avoided*.

Chapter TODO time- and event-driven are strong evidence that our claim that pure FP has indeed its place in ABS is valid - especially a full implementation in Sugarscape is a highly complex and non-trivial matter and our highly structured and robust approach can be seen as proof of success. At the same time we conclude that it is yet too early to pick up this paradigm for ABS. We think that engineering a proper implementation of a complex ABS model takes substantial effort in pure FP due to different techniques required and due to its strong static type system (TODO: cite productivity). We believe that at the moment such an effort pays off only in cases of high-impact and large-scale simulations which results might have far-reaching consequences e.g. influence policy decisions. It is only there where the high requirements for reproducibility, robustness and correctness provided by FP are really needed. Still, we plan on distilling the developed techniques of the case-study into a general purpose ABS library. This should allow implementing models much easier and quicker, making the pure FP approach an attractive alternative for prototyping, opening the direction for a broad use of FP in the field of ABS.

This thesis established now the knowledge of how to engineer time- and event-driven ABS with complex state both in the agent and environment, main difficulty is direct agent-interaction (see macal classification into 4 types of ABS), compile-time guaranteed reproducibility, explicit handling of complex state (read only, read/write), concurrency explicit and limited to STM, very promising concurrency but direct agent-interactions main problem (erlang as a rescue?), main drawbacks: everything is explicit, performance.

Further, it deepened the understanding of the structure of agent based computation by expressing it in a pure functional context, leading to a deeper and more general understanding of agents, how they can be represented and whether they indeed map naturally to objects or not. This central question of whether they map naturally to objects or not, permeates the whole thesis and drives

it forward. The last chapter gave an in-depth discussion of that question and we see that objects indeed have their place in ABS but, as we have carefully explained, the question is what objects constitute. By approaching the problem from a (pure) functional perspective, we also arrived at a deeper and broader understanding of objects, not only restricted to the traditional OO definition of Java,C++ or Python. So we can say: *"Yes they map naturally to objects, but we have to be precise what constitutes objects."*. Whether they are newtypes, tuples, (G)ADTs, pure functions, monads, comonads, arrows, SFs, MSFs, Actors or OO objects. They are all valid ways of representing agents with varying degree of abstraction, flexibility and power and they all come with their benefit and drawbacks which have to be clearly understood together with the problem to solve. This thesis simply added a promising new tool to the family of existing ones and only time will tell whether this tool is indeed as valuable as hinted in this thesis.

In this section we briefly summarise the future research to undertake, other than the one already mentioned in various parts of this thesis, especially in the respective discussion sections.

13.1 Shallow encoding

Using arrowized FRP with pure Signal Functions as in Yampa and Monadic Stream Functions as in Dunai is only *one* approach to ABS [1]. As we have shown at length in this thesis, although it is a robust and maintainable approach with highly valuable and promising benefits, there are other potential approaches left unexplored.

A standard approach to encode a problem in Haskell is by designing an embedded domain specific language (EDSL) for that (domain) problem and then implement the problem at hand in this specifically designed language. One has to distinguish between a *deep* and *shallow* encoding: in the former one, the EDSL is expressed "deeply" using direct data-types and functions of the host language Haskell - our approach using SFs and MSFs is of this nature.

The shallow encoding approach on the other hand provides a language on top of the Host language, often expressed using ADTs (Algebraic Data Types) or GADT (Generalised ADTs) which are used to encode a problem as a data-structure - the execution of the problem is done by an interpreter which evaluates this data-structure and translates it to the semantics of the host language. An example of a shallow embedded EDSL is a language for mathematical expressions consisting of constants, multiplication and subtractions, which are represented as syntax trees and then translated into Haskell multiplication and subtraction to arrive at the final result.

The main benefit of a shallow encoding is that it allows to separate definition from implementation due to the separation of the EDSL and its interpretation. This allows to strictly separate implementation from specification, composes

[1] After all, my education and thinking was influenced by object oriented thinking for 15 years, so this could be also the case that I intuitionally arrive at such a solution again.

very well and thus should also be easy to test as mocking of parts is straightforward.

So called *Freer Monads* [131] allow to express such shallow EDSL. One big additional advantage of them is that they free one from the ordering of effects imposed through Monad Transformers as mentioned in (TODO introduction to monad transformers in background). Unfortunately, Freer Monads seem to be somewhere around 30 times slower than the equivalent MTL code with a complexity of $O(n^2)$ [2]. For IO bound problems like business applications, this is not a big deal but as already mentioned in the introduction, ABS are almost always not IO bound, so raw computation is all what counts and this is undoubtedly worse with Freer monads. Even although there seem to be a better encoding possible, which is about 2x slower than MTL [3] the fact that we are already performance limited in our deep encoding makes the Free Monads approach not very appealing [4]. Still, we expect that it will be highly interesting and valuable research with focus on deeper and stronger guarantees about correctness and testing than our deep encoding.

13.2 A general purpose library

For pure functional ABS to ever reach a larger audience and acceptance, it will need a lot of support, especially in the form of a well designed, easy to use, robust, correct, high quality Haskell Library. Designing and developing such a library is research on its own as it needs to combine all the separate concepts introduced in this thesis into one code base. We hope that from this development further insights into ABS in general and pure functional ABS in particular will emerge, which can then be published to the community.

13.3 Actor based ABS

One of the thesis fundamental conclusions is that the future of ABS lies in a functional, actor based concurrent approach. It required the full thesis to come to this conclusion thus this thesis only scratched the surface of the potential for actor based ABS as in Erlang or Cloud Haskell. We think that this topic deserves rigorous research as well as it is currently strongly neglected with only very few papers existing, which just scratch the surface. The idea seems compelling: functional programming with an actor language seems the way to do ABS in the future as it gives us almost all properties introduced in this thesis with the exception that agent interactions are a lot easier and naturally expressed.

There have been a few attempts on implementing the actor model in real programming languages where the most notable ones are Erlang and Scala. Erlang was created in 1986 by Joe Armstrong for Eriksson for developing distributed

[2] `https://reasonablypolymorphic.com/blog/freer-monads/`
[3] `https://reasonablypolymorphic.com/blog/too-fast-too-free/`
[4] `https://reasonablypolymorphic.com/blog/freer-yet-too-costly/`

high reliability software in telecommunications. It implements light-weight processes, which allows to spawn thousands of them without heavy memory overhead. The language saw some use in implementing ABS with notable papers being [42, 43, 155, 138, 17]

Scala is a modern mixed paradigm programming language, which also allows functional programming and also incorporates a library for the actor model. It also saw the use in the implementation of ABS with a notable paper [97] and ScalABM [5] which is alibrary for ABM in economics.

The paper of [89] gives an excellent overview over the strengths and weaknesses of agent-based software-engineering, which can be directly applied to both Erlang and Scala.

TODO: process calculi like CSP, CCS and Pi-Calculus become applicable here, which allow to actually *prove* the correctness of a specification. Due to the direct mapping of the process calculi languages to erlang we see this as highly promising, also in light of the weak performance.

Due to the very different approach and implications the actor model of concurrency implies, we don't explore it further and leave it for further research as it is beyond the focus of the thesis.

13.4 Dependent and linear types

We see this thesis as an intermediary and necessary step towards dependent types for which we first needed to understand the potential and limitations of a non-dependently typed pure functional approach in Haskell. Dependent types are extremely promising in functional programming as they allow us to express stronger guarantees about the correctness of programs and go as far as allowing to formulate programs and types as constructive proofs, which must be total by definition [152, 5, 4].

So far no research using dependent types in agent-based simulation exists at all. In our next paper we want to explore this for the first time and ask more specifically how we can add dependent types to our pure functional approach, which conceptual implications this has for ABS and what we gain from doing so. We plan on using Idris [25] as the language of choice as it is very close to Haskell with focus on real-world application and running programs as opposed to other languages with dependent types e.g. Agda and Coq.

We hypothesize that dependent types could help ruling out even more classes of bugs at compile time and encode invariants and model specifications on the type level, which implies that we don't need to test them using e.g. property-testing with QuickCheck. This would allow the ABS community to reason about a model directly in code. We think that a promising approach is to follow the work of [26, 55, 27] in which the authors utilize GADTs to implement an indexed monad, which allows to implementation correct-by-construction software.

We have already started to outline a few core principles in the Appendix B, but we conjecture that the true benefit is yet to be revealed.

[5] https://github.com/ScalABM

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Part VI:

Appendices

Appendices

Appendix A

Correct-By-Construction System Dynamics

In this section we step-by-step develop a correct-by-construction implementation. Note that the constant parameters *populationSize, infectedCount, contactRate, infectivity, illnessDuration* are defined globally and omitted for clarity.

Computing the dynamics of a SD model happens by integrating the time over the equations. So conceptually we treat our SD model as a continuous function which is defined over time = 0 -¿ infinity and at each point in time outputs the values of each stock. In the case of the SIR model we have 3 stocks: Susceptible, Infected and Recovered. Thus we start our implementation by defining the output of our SD function: for each time-step we have the values of the 3 stocks:

```
type SIRStep = (Time, Double, Double, Double)
```

Next we define our continuous SD function which we obviously make a signal function. It has no input, because a SD system is only defined in its own terms and parameters without external input and has as output the *SIRStep*. Thus we define the following function type:

```
sir :: SF () SIRStep
```

An SD model is fundamentally built on feedback: the values at time t depend on the previous step. Thus we introduce feedback in which we feed the last step into the next step. Yampa provides the *loopPre :: c → SF (a, c) (b, c) → SF a b* function for that. It takes an initial value and a feedback signal function which receives the input a and the previous (or initial) value of the feedback and has to return the output b and the new feedback value c. *loopPre* then returns simply a signal function from a to b with the feedback happening transparent in the feedback signal function. Our initial feedback value is the initial state of the SD model at $t = 0$. Further we define the type of the feedback signal function:

```
sir = loopPre (0, initSus, initInf, initRec) sirFeedback
  where
    initSus = populationSize - infectedCount
    initInf = infectedCount
    initRec = 0

    sirFeedback :: SF ((), SIRStep) (SIRStep, SIRStep)
```

The next step is to implement the feedback signal function. As input we get *(a, c)* where a is the empty tuple () because a SD simulation has no input, and c is the fed back *SIRStep* from the previous (initial) step. With this we have all relevant data so we can implement the feedback function. We first match on the tuple inputs and construct a signal function using *proc*:

```
    sirFeedback = proc (_, (_, s, i, _)) -> do
```

Now we define our flows which are *infection rate* and *recovery rate*. The formulas for both of them can be seen in equations TODO (refer to the differential equations). This directly translates into Haskell code:

```
      let infectionRate = (i * contactRate * s * infectivity) / populationSize
          recoveryRate  = i / illnessDuration
```

Next we need to compute the values of the three stocks, following the formulas of TODO (refer to the Integral formulas). For this we need the *integral* function of Yampa which integrates over a numerical input using the rectangle rule. Adding initial values can be achieved with the (¡¡) operator of arrowized programming. This directly translates into Haskell code:

```
      s' <- (initSus+) ^<< integral -< (-infectionRate)
      i' <- (initInf+) ^<< integral -< (infectionRate - recoveryRate)
      r' <- (initRec+) ^<< integral -< recoveryRate
```

We also need the current time of the simulation. For this we use Yampas *time* function:

```
      t <- time -< ()
```

Now we only need to return the output and the feedback value. Both types are the same thus we simply duplicate the tuple:

```
      returnA -< dupe (t, s', i', r')

    dupe :: a -> (a, a)
    dupe a = (a, a)
```

We want to run the SD model for a given time with a given Δt by running the *sir* signal function. To *purely* run a signal function Yampa provides the function *embed :: SF a b -¿ (a, [(DTime, Maybe a)]) -¿ [b]* which allows to run an SF for a given number of steps where in each step one provides the Δt and an input a. The function then returns the output of the signal function for each step. Note that the input is optional, indicated by *Maybe*. In the first step at $t = 0$, the initial a is applied and whenever the input is *Nothing* in subsequent steps, the last a which was not *Nothing* is re-used.

Δt	Susceptibles	Infected	Recovered	Max Infected
1.0	17.52	26.87	955.61	419.07 @ t = 51
0.5	23.24	25.63	951.12	399.53 @ t = 47.5
0.1	27.56	24.27	948.17	384.71 @ t = 44.7
$1e-2$	28.52	24.11	947.36	381.48 @ t = 43.97
$1e-3$	28.62	24.08	947.30	381.16 @ t = 43.9
AnyLogic	28.625	24.081	947.294	381.132 @ t = 44

Table A.1: Results running the simulation with varying Δt until $t = 100$ with a population Size $N = 1{,}000$, contact rate $\beta = \frac{1}{5}$, infection probability $\gamma = 0.05$, illness duration $\delta = 15$ and initially 1 infected agent.

```
runSD :: Time -> DTime -> [SIRStep]
runSD t dt = embed sir ((), steps)
  where
    steps = replicate (floor (t / dt)) (dt, Nothing)
```

A.1 Discussion

We claim that our implementation is correct-by-construction because the code *is* the model specification - we have closed the gap between the specification and its implementation. Also we can guarantee that no non-deterministic influences can happening, neither in our nor Yampas library code due to the strong static type system of Haskell. This guarantees that repeated runs of the simulation will always result in the exact same dynamics given the same initial parameters, something of fundamental importance in System Dynamics.

A.1.1 Results

Although we have translated our model specifications directly into code we still we need to validate the dynamics and test the system for its numerical behaviour under varying Δt. This is necessary because numerical integration, which happens in the *integral* function, can be susceptible to instability and errors. Yampa implements the simple rectangle-rule of numerical integration which requires very small Δt to keep the errors minimal and arrive at sufficiently good results.

We have run the simulation with varying Δt to show what difference varying Δt can have on the simulation dynamics. We ran the simulations until $t = 100$ with a population Size $N = 1{,}000$, contact rate $\beta = \frac{1}{5}$, infection probability $\gamma = 0.05$, illness duration $\delta = 15$ and initially 1 infected agent. For comparison we looked at the final values at $t = 100$ of the susceptible, infected and recovered stocks. Also we compare the time and the value when the infected stock reaches its maximum. The values are reported in the Table A.1.

As additional validation we added the results of a System Dynamics simulation in AnyLogic Personal Learning Edition 8.3.1, which is reported in the

last row in the Table A.1. Also we provided a visualisation of the AnyLogics simulation dynamics in Figure A.1a. By comparing the results in Table A.1 and the dynamics in Figure A.1a to A.1b we can conclude that we arrive at the same dynamics, validating the correctness of our simulation also against an existing, well-known and established System Dynamics software package.

A.2 Conclusion

In this paper we have shown how to implement System Dynamics in a way that the resulting implementation is correct-by-construction, where the gap between the formal model specifications and the actual implementation in code is closed. We used the pure functional programming language Haskell for it and built on the Functional Reactive Programming concept to express our continuous-time simulation. The provided abstractions of Haskell and Functional Reactive Programming allowed to close the gap between the specification and implementation and further guarantee the absence of non-deterministic influences already at compile-time, making our correct-by-construction claims even stronger.

Further we showed the influence of different Δt and validated our implementation against the industry-strength System Dynamics simulation package AnyLogic Personal Learning Edition 8.3.1 where we could match our results with the one of AnyLogic, proving the correctness of our system also on the dynamics level.

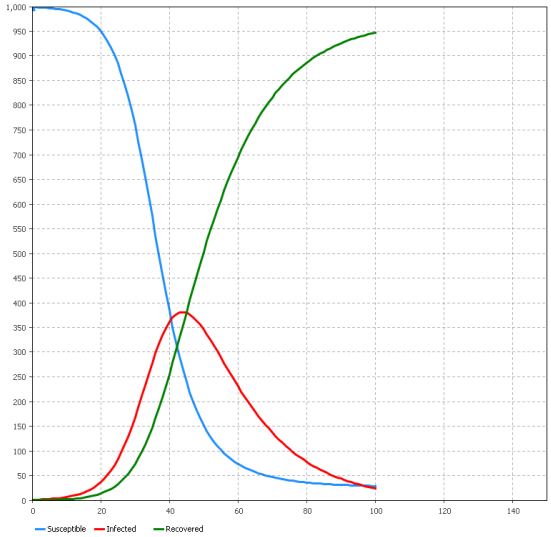
Obviously the numerical well behaviour depends on the integral function which uses the rectangle rule. We showed that for the SIR model and small enough Δt, the rectangle rule works well enough. Still it might be of benefit if we provide more sophisticated numerical integration like Runge-Kutta methods. We leave this for further research.

The key strength of System Dynamic simulation packages is their visual representation which allows non-programmers to express System Dynamics models and simulate them. We believe that one can auto-generate Haskell code using our approach to implement System Dynamics from such diagrams but leave this for further research.

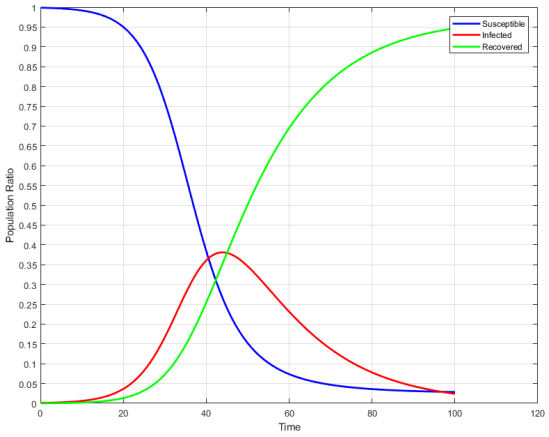
Also we are very well aware that due to the vast amount of visual simulation packages available for System Dynamics, there is no big need for implementing such simulations directly in code. Still we hope that our pure functional approach with Functional Reactive Programming might spark an interest in approaching the implementation of System Dynamics from a new perspective, which might lead to pure functional back-ends of visual simulation packages, giving them more confidence in their correctness.

A.3 Full Code

```
populationSize :: Double
populationSize = 1000
```



(a) System Dynamics simulation of SIR compartment model in AnyLogic Personal Learning Edition 8.3.1. Population Size $N = 1{,}000$, contact rate $\beta = \frac{1}{5}$, infection probability $\gamma = 0.05$, illness duration $\delta = 15$ with initially 1 infected agent. Simulation run until $t = 100$.



(b) Dynamics of the SIR compartment model following this implementation. Population Size $N = 1{,}000$, contact rate $\beta = \frac{1}{5}$, infection probability $\gamma = 0.05$, illness duration $\delta = 15$ with initially 1 infected agent. Simulation run until $t = 150$. Plot generated from data by this Haskell implementation using Octave.

Figure A.1: Visual comparison of the SIR SD dynamics generated by AnyLogic and our implementation in Haskell.

```
infectedCount :: Double
infectedCount = 1

contactRate :: Double
contactRate = 5

infectivity :: Double
infectivity = 0.05

illnessDuration :: Double
illnessDuration = 15

type SIRStep = (Time, Double, Double, Double)

sir :: SF () SIRStep
sir = loopPre (0, initSus, initInf, initRec) sirFeedback
  where
    initSus = populationSize - infectedCount
    initInf = infectedCount
    initRec = 0

    sirFeedback :: SF ((), SIRStep) (SIRStep, SIRStep)
    sirFeedback = proc (_, (_, s, i, _)) -> do
      let infectionRate = (i * contactRate * s * infectivity) / populationSize
          recoveryRate  = i / illnessDuration

      t <- time -< ()

      s' <- (initSus+) ^<< integral -< (-infectionRate)
      i' <- (initInf+) ^<< integral -< (infectionRate - recoveryRate)
      r' <- (initRec+) ^<< integral -< recoveryRate

      returnA -< dupe (t, s', i', r')

    dupe :: a -> (a, a)
    dupe a = (a, a)

runSD :: Time -> DTime -> [SIRStep]
runSD t dt = embed sir ((), steps)
  where
    steps = replicate (floor (t / dt)) (dt, Nothing)
```

Appendix B

The Equilibrium-Totality Correspondence

TODO UNFINISHED BUT OPTIONAL - write NON-DEPENDENTLY TYPED ARGUMENT - NEEDS SUBSTANTIAL RESEARCH: IMPLEMENT A TOTAL SIR IMPLEMENTATION IN IDRIS - write a short intro into dependent types - the question will remain: does this chapter really belong in this thesis?

In the property-tests of Chapter 10 and 9.2 we limited the time an individual simulation is run to a random range between 0 and 50. In this context, the decision to do so was practical to guarantee that we will actually terminate as both the event- and time-driven implementations would run forever if no time- and/or event-limit is specified [1].

However, restricting the simulation to a time- and/or event-limit is not necessary in a correct SIR implementation because it *will* reach an equilibrium *within finite time* at which point the simulation can be terminated. This is the case as soon as there are no more infected agents: intuitively this is clear because only infected agents can lead to infections of susceptible agents which then make the transition to recovered after having gone through the infection phase. The infected agents themselves *will* recover within finite time. Thus we can conclude that a correct implementation of the SIR model must enter a steady state in finite time.

Using this informal reasoning, we change the property-test from Chapter 10 to encode this property implicitly.

```
prop_sir_invariants :: Positive Int     -- ^ beta, contact rate
                    -> Property         -- ^ gamma, infectivity in range (0,1)
                    -> Positive Double  -- ^ delta, illness duration
                    -> [SIRState]       -- ^ population
                    -> Property
prop_sir_invariants
```

[1] Note that the event-driven implementation would terminate if the event-queue is empty but in the case of the SIR this will never be the case due to susceptible agents keep scheduling *MakeContact*, resulting in an infinite stream of events.

```
  (Positive cor) (P inf) (Positive ild) as  = property (do
-- CHANGED: run the SIR simulation with UNRESTRICTED time
ret <- genSimulationSIR ss cor inf ild 0
-- CHANGED: take data as long as not in equilibrium
let ret' = takeWhile ((>0).snd3.snd) ret
-- check invariants and return result
return (sirInvariants (length as) ret')
```

Unfortunately this code is dangerous: generally, we cannot distinguish between a very long or infinitely running simulation. It might be the case that there is a bug in our implementation which would violate the property that all infected agents eventually recover, in which case *takeWhile* might run forever. This means that we cannot write a property-test, which could tell us whether this property holds or not for both our time- and event-driven implementations - it is in general non-computable. Obviously this is nothing new and was established in the 1930s through the work of Turing [153]. The question is now: what can we do about it?

The solution is to abandon the power of general recursion and Turing-completeness and switch to a different kind of pure functional programming language in which programs can be checked for totality by the compiler. These languages have a different kind of type system, called dependent types. Generally, dependent types add the following concepts to pure functional programming:

1. Totality and termination - A total function is defined in [28] as one that terminates with a well-typed result or produces a non-empty finite prefix of a well-typed infinite result in finite time. In dependently typed languages which abandon Turing completeness this can be checked at compile time under certain circumstances.

2. Types are first-class citizen - In dependently typed languages, types can depend on any *values*, and can be *computed* at compile-time which makes them first-class citizen. This allows to compute the return type of a function depending on its input values. Note that this requires totality, otherwise type-checking would non-decidable and potentially non-terminating.

3. Types as *constructive* proofs - Because types can depend on any values and can be computed at compile-time, they can be used as constructive proofs (see B.2) which must terminate, this means a well-typed program (which is itself a proof) is always terminating which in turn means that it must consist out of total functions.

There exist a number of excellent introduction to dependent types which we use as main ressources for this section: [152, 129, 144, 28, 125]. We are using Idris [25] as the language of choice as it is very close to Haskell with focus on real-world application and running programs as opposed to other languages with dependent types e.g. Agda and Coq which serve primarily as proof assistants.

Dependent types are a very powerful addition to functional programming as they allow us to express even stronger guarantees about the correctness of

programs *already at compile-time*. They go as far as allowing to formulate programs and types as constructive proofs which must be *total* by definition [152, 5, 4].

So far no research using dependent types in agent-based simulation exists at all. We have already started to explore this for the first time and ask more specifically how we can add dependent types to our functional approach, which conceptual implications this has for ABS and what we gain from doing so. We are using Idris [25] as the language of choice as it is very close to Haskell with focus on real-world application and running programs as opposed to other languages with dependent types e.g. Agda and Coq which serve primarily as proof assistants.

We hypothesise, that dependent types will allow us to push the correctness of agent-based simulations to a new, unprecedented level by narrowing the gap between model specification and implementation. The investigation of dependent types in ABS will be the main unique contribution to knowledge of my Ph.D.

There is a strong relation between property-based tests and dependent types: in property-based testing we express specifications / properties / laws in code and test their invariance at run-time by random sampling the space. In dependent-types it is possible to express such properties already statically in types. This is the subject of the next part of the thesis which tries to move towards dependent types in ABS.

B.1 A total SIR implementation

In this section we want to implement a total agent-based SIR simulation, where the termination does NOT depend on time (is not terminated after a finite number of time-steps, which would be trivial).

Dependent Types and Idris' ability for totality- and termination-checking should theoretically allow us to proof that an agent-based SIR implementation terminates after finite time: if an implementation of the agent-based SIR model in Idris is total it is a formal proof by construction. Note that such an implementation should not run for a limited virtual time but run unrestricted of the time and the simulation should terminate as soon as there are no more infected agents, returning the termination time as an output. Also if we find a total implementation of the SIR model and extend it to the SIR+S model, which adds a cycle from Recovered back to Susceptible, then the simulation should become again non-total as reasoned above.

The HOTT book [129] states that lists, trees,... are inductive types/inductively defined structures where each of them is characterized by a corresponding *induction principle*. Thus, for a constructive proof of the totality of the agent-based SIR model we need to find the induction principle of it. This leaves us with the question of what the inductive, defining structure of the agent-based SIR model is? Is it a tree where a path through the tree is one way through the simulation

or is it something else? It seems that such a tree would grow and then shrink again e.g. infected agents. Can we then apply this further to (agent-based) simulation in general?

By this reasoning, a non-total, correctly implemented agent-based simulations of the SIR model will eventually terminate (note that this is independent of which environment is used and which parameters are selected). Still this does not formally proof that the agent-based approach itself will terminate and so far no formal proof of the totality of it was given.

Thus an agent-based implementation of the SIR simulation has to terminate if it is implemented correctly because all infected agents will recover after a finite number of steps after then the dynamics will be in equilibrium. Thus we have the following conditions for totality:

1. The simulation shall be terminated when there are no more infected agents.
2. All infected agents will recover after a finite number of time, which means that the simulation will eventually run out of infected agents.

   Unfortunately this criterion alone does not suffice because when we look at the SIR+S model, which adds a cycle from Recovered back to Susceptible, we have the same termination criterion, but we cannot guarantee that it will run out of infected. We need an additional criteria.
3. The source of infected agents is the pool of susceptible agents which is monotonic decreasing (not strictly though!) because recovered agents do NOT turn back into susceptibles.
4. finite number of initial susceptibles
5. finite number of initial infected
6. finite illness duration
7. finite contact rate

A central question in tackling this is whether to follow a model- or an agent-centric approach. The former one looks at the model and its specifications as a whole and encodes them e.g. one tries to directly find a total implementation of an agent-based model. The latter one looks only at the agent level and encodes that as dependently typed as possible and hopes that model guarantees emerge on a meta-level - put otherwise: does the totality of an implementation emerge when we follow an agent-centric approach?

B.2 Constructivism in ABS

The main theoretical and philosophical underpinnings of dependent types as in Idris are the works of Martin-Löf intuitionistic type theory. The view of dependently typed programs to be proofs is rooted in a deep philosophical discussion on the foundations of mathematics, which revolve around the existence

of mathematical objects, with two conflicting positions known as classic vs. constructive [2]. In general, the constructive position has been identified with realism and empirical computational content where the classical one with idealism and pragmatism.

In the classical view, the position is that to prove $\exists x.P(x)$ it is sufficient to prove that $\forall x.\neg P(x)$ leads to a contradiction. The constructive view would claim that only the contradiction is established but that a proof of existence has to supply an evidence of an x and show that $P(x)$ is provable. In the end this boils down whether to use proof by contradiction or not, which is sanctioned by the law of the excluded middle which says that $A \vee \neg A$ must hold. The classic position accepts that it does and such proofs of existential statements as above, which follow directly out of the law of the excluded middle, abound in mathematics [3]. The constructive view rejects the law of the excluded middle and thus the position that every statement is seen as true or false, independently of any evidence either way. [152] (p. 61): *The constructive view of logic concentrates on what it means to prove or to demonstrate convincingly the validity of a statement, rather than concentrating on the abstract truth conditions which constitute the semantic foundation of classical logic.*

To prove a conjunction $A \wedge B$ we need prove both A and B, to prove $A \vee B$ we need to prove one of A, B and know which we have proved. This shows that the law of the excluded middle can not hold in a constructive approach because we have no means of going from a proof to its negation. Implication $A \Rightarrow B$ in constructive position is a transformation of a proof A into a proof B: it is a function which transforms proofs of A into proofs of B. The constructive approach also forces us to rethink negation, which is now an implication from some proof to an absurd proposition (bottom): $A \Rightarrow \bot$. Thus a negated formula has no computational context and the classical tautology $\neg\neg A \Rightarrow A$ is then obviously no longer valid. Constructively solving this would require us to be able to effectively compute / decide whether a proposition is true or false - which amounts to solving the halting problem, which is not possible in the general case.

A very important concept in constructivism is that of finitary representation / description. Objects which are infinite e.g. infinite sets as in classic mathematics, fail to have computational computation, they are not computable. This leads to a fundamental tenet in constructive mathematics: [152] (p. 62): *Every object in constructive mathematics is either finite [..] or has a finitary description*

Concluding, we can say that constructive mathematics is based on principles quite different from classical mathematics, with the idealistic aspects of the latter replaced by a finitary system with computational content. Objects like functions are given by rules, and the validity of an assertion is guaranteed by a proof from which we can extract relevant computational information, rather than on idealist semantic principles.

All this is directly reflected in dependently typed programs as we introduced

[2] We follow the excellent introduction on constructive mathematics [152], chapter 3.

[3] Polynomial of degree n has n complex roots; continuous functions which change sign over a compact real interval have a zero in that interval,...

above: functions need to be total (finitary) and produce proofs like in *checkEqNat* which allows the compiler to extract additional relevant computational information. Also the way we described the (infinite) natural numbers was in an finitary way. In the case of decidable equality, the case where it is not equal, we need to provide an actual proof of contradiction, with the type of Void which is Idris representation of $\bot$.

B.2.1 Verification, Validation and Dependent Types

Dependent types allow to encode specifications on an unprecedented level, narrowing the gap between specification and implementation - ideally the code becomes the specification, making it correct-by-construction. The question is ultimately how far we can formulate model specifications in types - how far we can close the gap in the domain of ABS. Unless we cannot close that gap completely, to arrive at a sufficiently confidence in correctness, we still need to test all properties at run-time which we cannot encode at compile-time in types.

Nonetheless, dependent types should allow to substantially reduce the amount of testing which is of immense benefit when testing is costly. Especially in simulations, testing and validating a simulation can often take many hours - thus guaranteeing properties and correctness already at compile time can reduce that bottleneck substantially by reducing the number of test-runs to make.

Ultimately this leads to a very different development process than in the established object-oriented approaches, which follow a test-driven process. There one defines the necessary interface of an object with empty implementations for a given use-case first, then writes tests which cover all possible cases for the given use-case. Obviously all tests should fail because the functionality behind it was not implemented yet. Then one starts to implement the functionality behind it step-by-step until no test-case fails. This means that one runs all tests repeatedly to both check if the test-case one is working on is not failing anymore and to make sure that old test-cases are not broken by new code. The resulting software is then trusted to be correct because no counter examples through test hypotheses, could be found. The problem is: we could forget / not think of cases, which is the easier the more complex the software becomes (and simulations are quite complex beasts). Thus in the end this is a deductive approach.

With pure functional programming and dependent types the process is now mostly constructive, type-driven (see [28]). In that approach one defines types first and is then guided by these types and the compiler in an interactive fashion towards a correct implementation, ensured at compile-time. As already noted, the ABS methodology is constructive in nature but the established object-oriented test-driven implementation approach not as much, creating an impedance mismatch. We expect that a type-driven approach using dependent types reduces that mismatch by a substantial amount. Models like the Sugarscape are exploratory in nature and don't have a formal ground truth where one could derive equilibria or dynamics from and validate with. In such models the researchers work with informal hypotheses which they express be-

fore running the model and then compare them informally against the resulting dynamics.

It would be of interest if dependent types could be made of use in encoding hypotheses on a more constructive and formal level directly into the implementation code. So far we have no idea how this could be done but it might be a very interesting application as it allows for a more formal and automatic testable approach to hypothesis checking.

Note that *validation* is a different matter here: independent of our implementation approach we still need to validate the simulation against the real-world / ground-truth. This obviously requires to run the full simulation which could take up hours in either programming paradigm, making them absolutely equal in this respect. Also the comparison of the output to the real-world / ground-truth is completely independent to the paradigm. The fundamental difference happens in case of changes made to the code during validation: in case of the established test-driven object-oriented approach for every minor change one (should) re-run all tests, which could take up a substantial amount of additional time. Using a constructive, type-driven approach this is dramatically reduced and can often be completely omitted because the correctness of the change can be either guaranteed in the type or by informally reasoning about the code.

ABS as a constructive / generative science, follows Poperian approach of falsification: we try to construct a model which explains a real-world (empirical) phenomenon - if validation shows that the generated dynamics match the ones of the real-world sufficiently enough, we say that we have found *a* hypothesis (the model) which emergent properties explains the real-world phenomenon sufficiently enough. This is not a proof but only one possible explanation which holds for now and might be falsified in the future.

When we implement our simulation things change a bit as we add another layer: the conceptual model, describing the phenomenon, which is an abstraction of reality. This description can be of many forms but can be regarded on a line between completely formal (economic models) to informal (sociology) but the implementation will follow that description. The fundamental difference here is that in this case we want our implementation to be exactly the same as the conceptual model. Contrary to the real-world, where it is not possible to find a *true* model (as was argued by Popper), on this level we actually can construct an implementation which matches the conceptual model exactly because we have a description of the conceptual model. In the end we transform the conceptual model description in code, which is itself a formal description. In this translation process (speak: implementation / programming), one can make an endless number of mistakes. Generally we can distinguish between two classes of mistakes: 1) conceptual mistakes - wrong translation of the model specifications into code due to various reasons e.g. imprecise description, human error. The more precise an unambiguous a model description is, the less probable conceptual mistakes will be. 2) internal mistakes - normal programming mistakes e.g. access of arrays out of bounds, ... also using correlated Random Number generators. Level 0: Real-World phenomenon Level 1: Conceptual model of the real-world phenomenon Level 2: Implementation of the conceptual model Note

that we must speak of falsification and constructiveness on two different levels: - validation level: do the results of the conceptual model match the real-world phenomenon? the conceptual model is the hypothesis which says that its mechanics are sufficient to generate / construct the real-world phenomenon. At this level we are not interested in the implementation level anymore - the implemented model *is* (seen as) the conceptual model, and one only compares its output to the real-world. If the dynamics match, then we got a valid hypothesis which works for now. If the dynamics do NOT match, then the hypothesis (the model) is falsified and one needs to adjust / change the hypothesis (model). The validation will happen by tests, there is no other way, we have no formal specification of the real-world, we can only observe empirically the phenomena, so we run tests which try to falsify the outputs of the model: assuming it will generate phenomena of the real-world and test if it does. - implementation & verficiation level: in this step we are matching the code to the conceptual model. Here we are not only restricted to a test-driven approach because we have a more or less formal description of the conceptual model which we directly encode in our programming language. If the language allows to express model specifications already at compile-time then this means that the implementation narrows the gap between model specification and implementation which means it does not need to be tested at run-time because it is guaranteed for all inputs for all time.

The constructiveness of ABS and impendance mismatch: ABS methodology is constructive but the established implementation approach not too much, creating an impedance mismatch. this is especially visible in the test-driven development dependent types constructive nature could close this mismatch.

B.3 Discussion

In this chapter we have shown how to encode equilibria properties in the types in a way that the simulation automatically terminates when they are reached. This results then in a *total* simulation, creating a *correspondence between the equilibrium of a simulation and the totality of its implementation.* Of course this is only possible for models in which we know about their equilibria a priori or in which we can reason somehow that an equilibrium exists.

Models like the Sugarscape are exploratory in nature and don't have a formal ground truth where one could derive equilibria or dynamics from and validate with. In such models the researchers work with informal hypotheses which they express before running the model and then compare them informally against the resulting dynamics.

It would be of interest if dependent types could be made of use in encoding hypotheses on a more constructive and formal level directly into the implementation code. So far we have no idea how this could be done but it might be a very interesting application as it allows for a more formal and automatic testable approach to hypothesis checking.

Often, Agent-Based Models define their agents in terms of state-machines. It is easy to make wrong state-transitions e.g. in the SIR model when an infected

agent should recover, nothing prevents one from making the transition back to susceptible.

Using dependent types it might be possible to encode invariants and state-machines on the type level which can prevent such invalid transitions already at compile-time. This would be a huge benefit for ABS because of the popularity of state-machines in agent-based models.

State-Machines often have timed transitions e.g. in the SIR model, an infected agent recovers after a given time. Nothing prevents us from introducing a bug and *never* doing the transition at all.

With dependent types we might be able to encode the passing of time in the types and guarantee on a type level that an infected agent has to recover after a finite number of time steps. Also can dependent types be used to express the flow of time and that it is strongly monotonic increasing?

In more sophisticated models agents interact in more complex ways with each other e.g. through message exchange using agent IDs to identify target agents. The existence of an agent is not guaranteed and depends on the simulation time because agents can be created or terminated at any point during simulation.

Dependent types could be used to implement agent IDs as a proof that an agent with the given id exists *at the current time-step*. This also implies that such a proof cannot be used in the future, which is prevented by the type system as it is not safe to assume that the agent will still exist in the next step.

In case of an SD this will take forever to reach 0 due to the dynamics of the equations and floating point arithmetic is another difficulty. On the other hand, due to ABS discrete nature this is not an issue anymore: agents are discrete and as soon as we hit 0 infected agents - which, due to Integer representation, can be exact - an equilibrium is reached.

Note that there exists a SIR+S model, which adds a cycle back from Recovered to Susceptible - if we add this cycle in our total implementation, this should make it immediately non-total as an important criteria for totality gets violated: the source of susceptible is not finite anymore and we might run in non-stationary cycles like in a prey-predator model with Lotka-Volterra equations.

TODO: connect to property-based testing and put emphasise on the constructive nature and hypothesis testing: this is a popperian approach.

FP is the first step towards a more structural understanding of ABS implementations where dependent types should allow us to develop this even further. we leave this for further research and outline only broadly the ideas we want to follow.

Linear and Dependent Types with Idris 2: more general ideas / hints / research on how it is applicable to ABS

By definition, ABS is of constructive nature, as described by Epstein [47]: "If you can't grow it, you can't explain it" - thus an agent-based model and the simulated dynamics of it is itself a constructive proof which explain a real-world phenomenon sufficiently well. Although Epstein certainly wasn't talking about a constructive proof in any mathematical sense in this context (he was using the

word *generative*), dependent types *might* be a perfect match and correspondence between the constructive nature of ABS and programs as proofs.

When we talk about dependently typed programs to be proofs, then we also must attribute the same to dependently typed agent-based simulations, which are then constructive proofs as well. The question is then: a constructive proof of what? It is not entirely clear *what we are proving* when we are constructing dependently typed agent-based simulations. Probably the answer might be that a dependently typed agent-based simulation is then indeed a constructive proof in a mathematical sense, explaining a real-world phenomenon sufficiently well - we have closed the gap between a rather informal constructivism as mentioned above when citing Epstein who certainly didn't mean it in a constructive mathematical sense, and a formal constructivism, made possible by the use of dependent types.

Appendix C

Validating Sugarscape in Haskell

In this chapter we look at how property-based testing can be made of use to verify the *exploratory* Sugarscape model [49] as already introduced in Chapter 2.2.2. Whereas in the chapters on testing the explanatory SIR model we had an analytical solution, the fundamental difference in the exploratory Sugarscape model is that none such analytical solutions exist. This raises the question, which properties we can actually test in such a mode.

The answer lies in the very nature of exploratory models: they exist to explore and understand phenomena of the real world. Researchers come up with a model to explain the phenomena and then (hopefully) come up with a few questions and *hypotheses* about the emergent properties. The actual simulation is then used to test and refine the hypotheses. Indeed, descriptions, assumptions and hypotheses of varying formal degree abound in the Sugarscape model. Examples are: *the carrying capacity becomes stable after 100 steps; when agents trade with each other, after 1000 steps the standard deviation of trading prices is less than 0.05; when there are cultures, after 2700 steps either one culture dominates the other or both are equally present.*

We show how to use property-testing to formalise and check such hypotheses. For this purpose we undertook a full *verification* of our implementation [1] from Chapter 2.2.2. We validated it against the book [49] and a NetLogo implementation [161] [2].

[1] The code can be accessed freely from `https://github.com/thalerjonathan/phd/tree/master/public/towards/SugarScape/sequential`

[2] `https://www2.le.ac.uk/departments/interdisciplinary-science/research/replicating-sugarscape`, Note that lending didn't properly work in their NetLogo code and that they didn't implement Combat

C.1 Property-Based Hypothesis Testing

The property we test for is whether *the emergent property / hypothesis under test is stable under replicated runs* or not. To put it more technical, we use QuickCheck to run multiple replications with the same configuration but with different random-number streams and require that the tests all pass. During the verification process we have derived and implemented property-tests for the following hypotheses:

1. Disease Dynamics all recover - When disease are turned on, if the number of initial diseases is 10, then the population is able to rid itself completely from all disease within 100 ticks.

2. Disease Dynamics minority recover - When disease are turned on, if the number of initial diseases is 25, the population is not able to rid itself completely from all diseases within 1,000 ticks.

3. Trading Dynamics - When trading is enabled, the trading prices stabilise after 1,000 ticks with the standard deviation of the prices having dropped below 0.05.

4. Cultural Dynamics - When having two cultures, red and green, after 2,700 ticks, either the red or the blue culture dominates or both are equally strong. If they dominate they make up 95% of all agents, if they are equally strong they are both within 45% - 55%.

5. Inheritance Gini Coefficient - According to the book, when agents reproduce and can die of age then inheritance of their wealth leads to an unequal wealth distribution measured using the Gini Coefficient *averaging* at 0.7.

6. Carrying Capacity - When agents don't mate nor can die from age (chapter II), due to the environment, there is an *average* maximum carrying capacity of agents the environment can sustain. The capacity should be reached after 100 ticks and should be stable from then on.

7. Terracing - When resources regrow immediately, after a few steps the simulation becomes static. Agents will stay on their terraces and will not move any more because they have found the best spot due to their behaviour. About 45% will be on terraces and 95% - 100% are static and not moving any more.

The hypotheses and their validation is described more in-depth in the section C.2 below.

C.1.1 Implementation

To start with, we implement a custom data-generator to produce output from a Sugarscape simulation. The generator takes the number of ticks and the

scenario with which to run the simulation and returns a list of outputs, one for each tick.

```
sugarscapeUntil :: Int                -- ^ Number of ticks to run
                -> SugarScapeScenario -- ^ Scenario to run
                -> Gen [SimStepOut]   -- ^ Output of each step
sugarscapeUntil ticks params = do
  -- create a random-number generators
  g <- genStdGen
  -- initialise the simulation state with the given random-number generator
  -- and the parameters
  let (simState, _, _) = initSimulationRng g params
  -- run the simulation with the given state for number of ticks
  return (simulateUntil ticks simState)
```

Using this generator, we can very conveniently produce sugarscape data within a property. Depending on the problem, we can generate only a single run or multiple replications, in case the hypothesis is assuming *averages*. To see its use, we show the encoding of the *Disease Dynamics (1)* hypothesis. Its type is *Property*, which is required by QuickChecks top-level testing function. To generate a property, the *property* function is used which takes a *Gen Bool* computation or a simple *Bool* function as predicate to indicate success (True) or failure (False).

```
prop_disease_allrecover :: Property
prop_disease_allrecover = property (do
  -- after 100 ticks...
  let ticks  = 100
  -- ... given Animation V-1 parameter configuration ...
  let params = mkParamsAnimationV_1
  -- ... from 1 sugarscape simulation ...
  aos <- sugarscapeLast ticks params
  -- ... counting all infected agents ...
  let infected = length (filter (==False)) map (null . sugObsDiseases . snd) aos
  -- ... should result in all agents to be recovered
  return (cover 100 (infected == 0) "Diseases all recover" True)
```

From the implementation it becomes clear, that this hypothesis states that the property has to hold *for all* replications. The *Inheritance Gini Coefficient (5)* hypothesis on the other hand assumes that the Gini Coefficient *averages* at 0.7. We cannot average over replicated runs of the same property thus we generate multiple replications of the sugarscape data within the property and employ a two-sided T-Test with a 95% confidence to test the hypothesis:

```
prop_gini :: Int      -- ^ Number of replications
          -> Double   -- ^ Confidence of the t-test
          -> Property
prop_gini repls confidence = property (do
  -- after 1000 ticks...
  let ticks = 1000
  -- ... the gini coefficient should average at 0.7 ...
  let expGini = 0.7
  -- ... given the Figure III-7 parameter configuration ...
  let params = mkParamsFigureIII_7
```

```
-- ... from 100 replications ...
gini <- vectorOf repls (genGiniCoeff ticks params)
-- on a two-tailed t-test with given confidence
let giniTTest = tTestSamples TwoTail expGini (1 - confidence) gini
return giniTTest
```

C.1.2 Running the tests

As already pointed out, QuickCheck tries to run by default up to 100 replications of a property and if all evaluate to *True* the property-test succeeds. On the other hand, QuickCheck will stop at the first predicate which evalutes to *False* and marks the whole property-test as failed, no matter how many replications got through already. For this reason we have used *cover* with an expected percentage of 100, meaning that we expect all tests to fall into the coverage class.

Due to the duration even 1,000 ticks can take to compute, to get a first estimate of our hypotheses tests within reasonable time, we reduce the number of maximum successful replications required to 10 and when doing T-tests 10 replications are run there as well.

```
SugarScape Tests
  Disease Dynamics All Recover:      OK (29.25s)
    +++ OK, passed 10 tests (100% Diseases all recover).

  Disease Dynamics Minority Recover: OK (536.00s)
    +++ OK, passed 10 tests (100% Diseases no recover).

  Trading Dynamics:                  OK (149.33s)
    +++ OK, passed 10 tests (70% Prices std less than 5.0e-2).
    Only 70% Prices std less than 5.0e-2, but expected 100%

  Cultural Dynamics:                 OK (996.84s)
    +++ OK, passed 10 tests (50% Cultures dominate or equal).
    Only 50% Cultures dominate or equal, but expected 100%

  Carrying Capacity:   OK (988.20s)
    +++ OK, passed 10 tests (90% Carrying capacity averages at 204.0).
    Only 90% Carrying capacity averages at 204.0, but expected 100%

  Terracing:           OK (280.59s)
    +++ OK, passed 10 tests (80% Terracing is happening).
    Only 80% Terracing is happening, but expected 100%

  Inheritance Gini:    OK (7232.59s)
    +++ OK, passed 0 tests (0% Gini coefficient averages at 0.7).
    Only 0% Gini coefficient averages at 0.7, but expected 100%
```

How to deal with the failure of the hypotheses is obviously highly model specific. A first approach is to increase the number of replications to run to 100

to get a more robust estimate of the failure rate. If the failure rate stays within reasonable ranges then one can arguably assume that the hypothesis is valid for sufficiently enough cases. On the other hand, if the failure rate escalates, then it is reasonable to deem the hypothesis invalid and refine it or even abandon it altogether.

With the exception of the Gini Coefficient, we accept the failure rate of the hypotheses we presented here and deem them sufficiently valid for the task at hand. In case of the Gini Coefficient, none of the replication was successful, which makes it obvious that it does *not* average at 0.7. Thus the hypothesis as stated in the book does not hold and is invalid. One way to deal with it would be to simply delete it. Another, more constructive approach, is to keep it but require all replications to fail by marking it with *expectFailure* instead of *property*. In this way an invalid hypothesis is marked explicitly and acts as documentation and also as test.

C.2 Hypotheses and test-cases

C.2.1 Terracing

Our implementation reproduces the terracing phenomenon as described on page TODO in Animation and as can be seen in the NetLogo implementation as well. We implemented a property-test in which we measure the closeness of agents to the ridge: counting the number of same-level sugars cells around them and if there is at least one lower then they are at the edge. If a certain percentage is at the edge then we accept terracing. The question is just how much, which we estimated from tests and resulted in 45%. Also, in the terracing animation the agents actually never move which is because sugar immediately grows back thus there is no incentive for an agent to actually move after it has moved to the nearest largest cite in can see. Therefore we test that the coordinates of the agents after 50 steps are the same for the remaining steps.

C.2.2 Carrying Capacity

Our simulation reached a steady state (variance ¡ 4 after 100 steps) with a mean around 182. Epstein reported a carrying capacity of 224 (page 30) and the NetLogo implementations' [161] carrying capacity fluctuates around 205 which both are significantly higher than ours. Something was definitely wrong - the carrying capacity has to be around 200 (we trust in this case the NetLogo implementation and deem 224 an outlier).

After inspection of the NetLogo model we realised that we implicitly assumed that the metabolism range is *continuously* uniformly randomized between 1 and 4 but this seemed not what the original authors intended: in the NetLogo model there were a few agents surviving on sugarlevel 1 which was never the case in ours as the probability of drawing a metabolism of exactly 1 is practically zero

when drawing from a continuous range. We thus changed our implementation to draw a discrete value as the metabolism.

This partly solved the problem, the carrying capacity was now around 204 which is much better than 182 but still a far cry from 210 or even 224. After adjusting the order in which agents apply the Sugarscape rules, by looking at the code of the NetLogo implementation, we arrived at a comparable carrying capacity of the NetLogo implementation: agents first make their move and harvest sugar and only after this the agents metabolism is applied (and ageing in subsequent experiments).

For regression-tests we implemented a property-test which tests that the carrying capacity of 100 simulation runs lies within a 95% confidence interval of a 210 mean. These values are quite reasonable to assume, when looking at the NetLogo implementation - again we deem the reported Carrying Capacity of 224 in the Book to be an outlier / part of other details we don't know.

One lesson learned is that even such seemingly minor things like continuous vs. discrete or order of actions an agent makes, can have substantial impact on the dynamics of a simulation.

C.2.3 Wealth Distribution

By visual comparison we validated that the wealth distribution (page 32-37) becomes strongly skewed with a histogram showing a fat tail, power-law distribution where very few agents are very rich and most of the agents are quite poor. We compute the skewness and kurtosis of the distribution which is around a skewness of 1.5, clearly indicating a right skewed distribution and a kurtosis which is around 2.0 which clearly indicates the 1st histogram of Animation II-3 on page 34. Also we compute the Gini coefficient and it varies between 0.47 and 0.5 - this is accordance with Animation II-4 on page 38 which shows a gini-coefficient which stabilises around 0.5 after. We implemented a regression-test testing skewness, kurtosis and gini-coefficients of 100 runs to be within a 95% confidence interval of a two-sided t-test using an expected skewness of 1.5, kurtosis of 2.0 and gini-coefficient of 0.48.

C.2.4 Migration

With the information provided by [161] we could replicate the waves as visible in the NetLogo implementation as well. Also we propose that a vision of 10 is not enough yet and shall be increased to 15 which makes the waves very prominent and keeps them up for much longer - agent waves are travelling back and forth between both Sugarscape peaks. We haven't implemented a regression-test for this property as we couldn't come up with a reasonable straight forward approach to implement it.

C.2.5 Pollution and Diffusion

With the information provided by [161] we could replicate the pollution behaviour as visible in the NetLogo implementation as well. We haven't implemented a regression-test for this property as we couldn't come up with a reasonable straight forward approach to implement it.

C.2.6 Mating

We could not replicate Figure III-1 (TODO: page) - our dynamics first raised and then plunged to about 100 agents and go then on to recover and fluctuate around 300. This findings are in accordance with [161], where they report similar findings - also when running their NetLogo code we find the dynamics to be qualitatively the same.

Also at first we weren't able to reproduce the cycles of population sizes. Then we realised that our agent-behaviour was not correct: agents which died from age or metabolism could still engage in mating before actually dying - fixing this to the behaviour, that agents which died from age or metabolism won't engage in mating solved that and produces the same swings as in [161]. Although our bug might be obvious, the lack of specification of the order of the application of the rules is an issue in the SugarScape book.

C.2.7 Inheritance

We couldn't replicate the findings of the Sugarscape book regarding the Gini coefficient with inheritance. The authors report that they reach a gini coefficient of 0.7 and above in Animation III-4. Our Gini coefficient fluctuated around 0.35. Compared to the same configuration but without inheritance (Animation III-1) which reached a Gini coefficient of about 0.21, this is indeed a substantial increase - also with inheritance we reach a larger number of agents of around 1,000 as compared to around 300 without inheritance. The Sugarscape book compares this to chapter II, Animation II-4 for which they report a Gini coefficient of around 0.5 which we could reproduce as well. The question remains, why it is lower (lower inequality) with inheritance?

The baseline is that this shows that inheritance indeed has an influence on the inequality in a population. Thus we deemed that our results are qualitatively the same as the make the same point. Still there must be some mechanisms going on behind the scenes which are unspecified in the original Sugarscape.

C.2.8 Cultural Dynamics

We could replicate the cultural dynamics of AnimationIII-6 / Figure III-8: after 2700 steps either one culture (red / blue) dominates both hills or each hill is dominated by a different ulture. We wrote a test for it in which we run the simulation for 2.700 steps and then check if either culture dominates with a ratio of 95% or if they are equal dominant with 45%. Because always a few

agents stay stationary on sugarlevel 1 (they have a metabolism of 1 and cant see far enough to move towards the hills, thus stay always on same spot because no improvement and grow back to 1 after 1 step), there are a few agents which never participate in the cultural process and thus no complete convergence can happen. This is accordance with [161].

C.2.9 Combat

Unfortunately [161] didn't implement combat, so we couldn't compare it to their dynamics. Also, we weren't able to replicate the dynamics found in the Sugarscape book: the two tribes always formed a clear battlefront where some agents engage in combat e.g. when one single agent strays too far from its tribe and comes into vision of the other tribe it will be killed almost always immediately. This is because crossing the sugar valley is costly: this agent wont harvest as much as the agents staying on their hill thus will be less wealthy and thus easier killed off. Also retaliation is not possible without any of its own tribe anywhere near.

We didn't see a single run where an agent of an opposite tribe "invaded" the other tribes hill and ran havoc killing off the entire tribe. We don't see how this can happen: the two tribes start in opposite corners and quickly occupy the respective sugar hills. So both tribes are acting on average the same and also because of the number of agents no single agent can gather extreme amounts of wealth - the wealth should rise in both tribes equally on average. Thus it is very unlikely that a super-wealthy agent emerges, which makes the transition to the other side and starts killing off agents at large. First: a super-wealthy agent is unlikely to emerge, second making the transition to the other side is costly and also low probability, third the other tribe is quite wealthy as well having harvested for the same time the sugar hill, thus it might be that the agent might kill a few but the closer it gets to the center of the tribe the less like is a kill due to retaliation avoidance - the agent will simply get killed by others.

Also it is unclear in case of AnimationIII-11 if the R rule also applies to agents which get killed in combat. Nothing in the book makes this clear and we left it untouched so that agents who only die from age (original R rule) are replaced. This will lead to a near-extinction of the whole population quite quickly as agents kill each other off until 1 single agent is left which will never get killed in combat because there are no other agents who could kill it - instead it will enter an infinite die and reborn cycle thanks to the R rule.

C.2.10 Spice

The book specifies for AnimationIV-1 a vision between 1-10 and a metabolism between 1-5. The last one seems to be quite strange because the maximum sugar / spice an agent can find is 4 which means that agents with metabolism of either 5 will die no matter what they do because the can never harvest enough to satisfy their metabolism. When running our implementation with this configuration the number of agents quickly drops from 400 to 105 and continues to slowly

degrade below 90 after around 1000 steps. The implementation of [161] used a slightly different configuration for AnimationIV-1, where they set vision to 1-6 and metabolism to 1-4. Their dynamics stabilise to 97 agents after around 500+ steps. When we use the same configuration as theirs, we produce the same dynamics. Also it is worth nothing that our visual output is strikingly similar to both the book AnimationIV-1 and [161].

C.2.11 Trading

For trading we had a look at the NetLogo implementation of [161]: there an agent engages in trading with its neighbours *over multiple rounds* until either MRSs cross over or no trade has happened anymore. Because [161] were able to exactly replicate the dynamics of the trading time-series we assume that their implementation is correct. We think that the fact that an agent interact with its neighbours over multiple rounds is made not very clear in the book. The only hint is found on page 102: *"This process is repeated until no further gains from trades are possible."* which is not very clear and does not specify exactly what is going on: does the agent engage with all neighbours again? is the ordering random? Another hint is found on page 105 where trading is to be stopped after MRS cross-over to prevent an infinite loop. Unfortunately this is missing in the Agent trade rule T on page 105. Additional information on this is found in footnote 23 on page 107. Further on page 107: *"If exchange of the commodities will not cause the agents' MRSs to cross over then the transaction occurs, the agents recompute their MRSs, and bargaining begins anew."*. This is probably the clearest hint that trading could occur over multiple rounds.

We still managed to exactly replicate the trading-dynamics as shown in the book in Figure IV-3, Figure IV-4 and Figure IV-5. The book is also pretty specific on the dynamics of the trading-prices standard-deviation: on page 109 the authors specify that at t=1000 the standard deviation will have always fallen below 0.05 (Figure IV-5), thus we implemented a property-test which tests for exactly that property. Unfortunately we didn't reach the same magnitude of the trading volume where ours is much lower around 50 but it is equally erratic, so we attribute these differences to other missing specifications or different measurements because the price-dynamics match that well already so we can safely assume that our trading implementation is correct.

According to the book, Carrying Capacity (Animation II-2) is increased by Trade (page 111/112). To check this it is important to compare it not against AnimationII-2 but a variation of the configuration for it where spice is enabled, otherwise the results are not comparable because carrying capacity changes substantially when spice is on the environment and trade turned off. We could replicate the findings of the book: the carrying capacity increases slightly when trading is turned on. Also does the average vision decrease and the average metabolism increase. This makes perfect sense: trading allows genetically weaker agents to survive which results in a slightly higher carrying capacity but shows a weaker genetic performance of the population.

According to the book, increasing the agent vision leads to a faster conver-

gence towards the (near) equilibrium price (page 117/118/119, Figure IV-8 and Figure IV-9). We could replicate this behaviour as well.

According to the book, when enabling R rule and giving agents a finite life span between 60 and 100 this will lead to price dispersion: the trading prices won't converge around the equilibrium and the standard deviation will fluctuate wildly (page 120, Figure IV-10 and Figure IV-11). We could replicate this behaviour as well.

The Gini coefficient should be higher when trading is enabled (page 122, Figure IV-13) - We could replicate this behaviour.

Finite lives with sexual reproduction lead to prices which don't converge (page 123, Figure IV-14). We could reproduce this as well but it was important to re-set the parameters to reasonable values: increasing number of agents from 200 to 400, metabolism to 1-4 and vision to 1-6, most important the initial endowments back to 5-25 (both sugar and spice) otherwise hardly any mating would happen because the agents need too much wealth to engage (only fertile when have gathered more than initial endowment). What was kind of interesting is that in this scenario the trading volume of sugar is substantially higher than the spice volume - about 3 times as high.

From this part, we didn't implement: Effect of Culturally Varying Preferences, page 124 - 126, Externalities and Price Disequilibrium: The effect of Pollution, page 126 - 118, On The Evolution of Foresight page 129 / 130.

C.2.12 Diseases

We were able to exactly replicate the behaviour of Animation V-1 and Animation V-2: in the first case the population rids itself of all diseases (maximum 10) which happens pretty quickly, in less than 100 ticks. In the second case the population fails to do so because of the much larger number of diseases (25) in circulation. We used the same parameters as in the book. The authors of [161] could only replicate the first animation exactly and the second was only deemed "good". Their implementation differs slightly from ours: In their case a disease can be passed to an agent who is immune to it - this is not possible in ours. In their case if an agent has already the disease, the transmitting agent selects a new disease, the other agent has not yet - this is not the case in our implementation and we think this is unreasonable to follow: it would require too much information and is also unrealistic. We wrote regression tests which check for animation V-1 that after 100 ticks there are no more infected agents and for animation V-2 that after 1000 ticks there are still infected agents left and they dominate: there are more infected than recovered agents.

C.3 Discussion

In this chapter we showed how to use QuickCheck to formalise and check hypotheses about an *exploratory* agent-based model, in which no ground truth exists. Due to ABS stochastic nature in general it became obvious that to

get a good measure of a hypotheses validity we need to allow failure using the *maxFailPercent* argument of QuickCheck. This allowed us to show that the hypotheses we have presented are sufficiently valid for the task at hand and can indeed be used for expressing and formalising emergent properties of the model and also as regression tests within a TDD cycle.