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PHD THESIS

The Pure Functional Programming Paradigm In Agent-Based Simulation

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Abstract

This thesis shows how to implement Agent-Based Simulations (ABS) using the *pure* functional programming paradigm and what the benefits and drawbacks are when doing so. As language of choice, Haskell is used due to its modern nature, increasing use in real-world applications and *pure* nature. The thesis presents various implementation techniques to ABS and then discusses concurrency and parallelism and verification and validation in ABS in a pure functional setting. Additionally the thesis briefly discusses the use of dependent types in ABS, to close the gap between specification and implementation - something the presented implementation techniques don't focus on. Finally a case-study is presented which tries to bring together the insights of the previous chapters by replicating an agent-based model both in pure and dependently typed functional programming. The agent-based model which was selected was much discussed in ABS communities as it claimed to have solved a fundamental problem of economics but it was then found that the implementation had a number of bugs which shed doubt on the validity and correctness of the results. The thesis' case study investigates whether this failure could have happened in pure and dependent functional programming and is a further test to see of how much value functional programming is to ABS.

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Chapter 1

Introduction

The traditional approach to Agent-Based Simulation (ABS) has so far always been object-oriented techniques, due to the influence of the seminal work of Epstein et al [13] 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* [27] which still holds up today.

This thesis challenges that metaphor and explores ways of approaching ABS with the *pure* functional programming paradigm using the languages Haskell and Idris. It is the first one to do so on a *systematical* level and develops a foundation by presenting fundamental concepts and advanced features to show how to leverage the benefits of both languages [19, 7] to become available when implementing ABS functionally. By doing this, the thesis both 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 thesis claims that the agent-based simulation 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.

Thus this thesis' general research question is *how to implement ABS purely functional and what the benefits and drawbacks are of doing so*. Further, it hypothesises that by using pure functional programming for implementing ABS makes it is easy to add parallelism and concurrency, the resulting simulations are easy to test and verify, applicable to property-based testing, 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.

1.1 Publications

Throughout the course of the Ph.D. four (4) papers were published:

1. The Art Of Iterating - Update Strategies in Agent-Based Simulation [36]
- This paper derives the 4 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.
2. Pure Functional Epidemics [35] - 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.
3. A Tale Of Lock-Free Agents (TODO cite) - 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. It does not go into technical details of functional programming as it is written for a simulation Journal.
4. Towards Pure Functional Agent-Based Simulation (TODO cite) - 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.

1.2 Contributions

1. 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 which were added to object-oriented languages in recent years, because of its established benefits in concurrent programming, testing and software-development in general, presenting such foundational research gives this thesis significant impact. Also it opens the way for the benefits of FP to incorporate into scientific computing, which are explored in the contributions below.
2. 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 FP because of retry-semantics can be guaranteed to exclude non-repeatable persistent side-effects already at compile time. 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. Due to the increasing need for massively large-scale ABS in recent years [22], making this possible within a purely functional approach as well, gives this thesis substantial impact.
3. This thesis is the first to present the use of property-based testing in ABS which allows a declarative specification- testing of the implemented ABS directly in code with *automated* 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. 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.

1.3 Thesis structure

This thesis focuses on a strong narrative which tells the story of *how* to do ABS with pure functional programming, *why* one would do so and when one should *avoid* this paradigm in ABS.

TODO: write when all is finished

Chapter 2

Literature Review

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 [11, 33, 21].

A multi-method simulation library in Haskell called *Aivika 3* is described in the technical report [32]. 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 [4] the author investigates Haskell's parallel and concurrency features to implement (amongst others) *HLogo*, a Haskell clone of the NetLogo [40] 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 an unrestricted context (known as *IO*) 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 can be seen as one of the first works on ABS using Haskell. Despite the concurrency and parallel aspect our work share, our approach is rather different: we avoid IO within the agents under all costs and explore the use of STM more on a conceptual level rather than implementing a ABS library and compare our case-studies with lock-based and imperative implementations.

There exists some research [12, 37, 31] using the functional programming language Erlang [2] 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 [41]. It emphasises message-passing concurrency with share-nothing semantics (no shared state be-

tween 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 [4] 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 [22] discusses a framework, which allows to map Agent-Based Simulations to Graphics Processing Units (GPU). Amongst others they use the SugarScape model [13] 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 we can draw inspiration from their work in terms of performance measurement and comparison of the SugarScape model.

Using functional programming for DES was discussed in [21] 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 [30, 38]. This language called FRABJOU 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 emerged out of Simula 67 [10] which was created for simulation purposes. Simula 67 already supported Discrete Event Simulation 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 [18]. While it has solved some issues related to implementing ABS in Haskell it still lacks a few important features necessary for ABS. We don't see any way of implementing an environment in Lustre as we do in our approach in Section ???. 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.

Research on TDD of ABS is quite new and thus there exist relative few pub-

lications. The work [9] is the first to discuss how to apply the TDD approach 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 [26] 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 [3] discusses a similar approach to DES in the AnyLogic software toolkit.

The paper [28] 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. This approach will become of importance later on in our SIR case study.

The paper [8] propose property-driven design of robot swarms. They propose a top-down approach by specifying properties a swarm of robots should have from which a prescriptive model is created, which properties are verified using model checking. Then a simulation is implemented following this prescriptive and verified model after then the physical robots are implemented. The authors identify the main difficulty of implementing such a system that the engineer must *"think at the collective-level, but develop at the individual-level"*. It is arguably true that this also applies to implementing agent-based models and simulations where the same collective-individual separation exists from which emergent system behaviour of simulations emerges - this is the very foundation of the ABS methodology.

The paper [17] 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 JUnit to run automated tests. To demonstrate their framework they provide also a case study of an agent-based simulation of synaptic connectivity where they provide an in-depth explanation of their levels of test together with code.

Although the work on TDD is scarce in ABS, there exists quite some research on applying TDD and unit-testing to multi-agent systems (MAS). Although MAS is a different discipline than ABS, the latter one has derived many technical concepts from the former one thus testing concepts applied to MAS might also be applicable to ABS. The paper [25] is a survey of testing in MAS. It distinguishes between unit tests which test units that make up an agent, agent tests which test the combined functionality of units that make up an agent, integration tests which test the interaction of agents within an environment and observe emergent behaviour, system test which test the MAS as a system running at the target

environment and acceptance test in which stakeholders verify that the software meets their goal. Although not all ABS simulations need acceptance and system tests, still this classification gives a good direction and can be directly transferred to ABS.

The authors of [5] 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 TODO 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 with arbitrary number synchronised agent-interactions.

The authors of [6] 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. As a remedy to having no related work to build on, we looked into works which apply dependent types to solve real world problems from which we then can draw inspiration from.

In his talk [34], 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 [16] defines computer-games as "[...] *soft real-time interactive agent-based computer simulations*" (p. 9) and in the end they have also very important 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. 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 parallelized easily in a pure functional language and updating game-objects concurrently using software transactional memory (STM).

Chapter 3

Methodology

This chapter introduces the background and methodology used in the following chapters. Roughly 50% exists already.

3.1 Agent-Based Simulation

History, methodology (what is the purpose of ABS: 3rd way of doing science: exploratory, helps understand real-world phenomena), classification according to [23], ABS vs. MAS, event- vs. time-driven [24], examples: agent-based SIR, SugarScape, Gintis Bartering

3.1.1 Traditional approaches

Introduce established implementation approaches to ABS. Frameworks: NetLogo, Anylogic, Libraries: RePast, DesmoJ. Programming: Java, Python, C++. Correctness: ad-hoc, manual testing, test-driven development.

3.1.2 Verification & Validation

Introduction Verification & Validation (V & V in the context of ABS).

3.2 Pure functional programming

Definition, Haskell references,

In our research we are using the *pure* functional programming language Haskell. The paper of [19] 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 main points why we decided to go for Haskell are:

- Rich Feature-Set - it has all fundamental concepts of the pure functional programming paradigm included. 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 [20, 19], is applicable to a number of real-world problems [29] and has a large number of libraries available ¹.
- 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.
- Purity - 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 (exceptions are when doing concurrency but there we restrict most of the concepts to STM).
- It is as close to pure functional programming, as in the lambda-calculus, as we want to get. Other languages are often a mix of paradigms and soften some criteria / are not strictly functional and have different purposes. Also Haskell is very strong rooted in Academia and lots of knowledge is available, especially at Nottingham, Lisp / Scheme was considered because it was the very first functional programming language but deemed to be not modern enough with lack of sufficient libraries. Also it would have given the Erlang was considered in prototyping and allows to map the messaging concept of ABS nicely to a concurrent language but was ultimately rejected due to its main focus on concurrency and not being purely functional. Scala was considered as well and has been used in the research on the Art Of Iterating paper but is not purely functional and can be also impure.

3.2.1 Functional Reactive Programming

Short introduction to FRP (yampa), based on my pure functional epidemics paper.

3.2.2 Monadic Stream Functions

Short introduction to MSFs (dunai), based on my pure functional epidemics paper.

¹https://wiki.haskell.org/Applications_and_libraries

3.3 Dependent Types

Example, Equality as Type, Philosophical Foundations: Constructive mathematics

Chapter 4

Pure Functional ABS

Is the main chapter of the thesis to discuss *how* can we do pure functional ABS.
Roughly 75% exists already.

4.1 Time-Driven ABS

Following pure functional ABS, also discuss how can we implement the 4 update-strategies of the art-iterating paper in our pure functional approach.

4.1.1 A hybrid approach

TODO: discuss using sdhaskell paper

4.1.2 Super-Sampling

discuss using FrABS report

4.2 Event-Driven ABS

Following towards papers SugarScape implementation

4.2.1 Synchronised Agent-Interactions

Following towards papers SugarScape implementation

Chapter 5

Parallelism and Concurrency

Establish how concurrency and parallelism can be made easily available in ABS using pure functional programming. Mostly follow STM paper and add pure parallelism in ABS. Make clear that Haskell allows to distinguish between pure, deterministic parallelism and impure, non-deterministic concurrency.

About 50% finished.

5.1 Adding Parallelism

Discusses where there is potential for adding parallelism: using data-parallel data-structures for the environment so cells can be updated in parallel, in time-driven ABS agents can be updated in parallel using `parMap` because they all act conceptually at the same time (and if they don't run in monadic code). 0% finished.

5.2 Adding Concurrency with STM

This is a shorter recap of the STM paper, 100% finished.

Chapter 6

Verification & Correctness

Exploring ways in which pure functional ABS can be of benefit to verification & validation and increasing correctness of an ABS implementation.

Roughly 50%

6.1 Using the Type-System

Static type system eliminates a large number run-time bugs.

6.2 Reasoning

TODO: can we apply equational reasoning? Can we (informally) reason about various properties e.g. termination?

6.3 Unit-Testing

Follow unit-testing of the whole simulation as prototyped for towards paper.

6.4 Property-Based Testing

Follow property-based testing as prototyped for towards paper. Also discuss property-based testing as explored in the SIR (time-driven) and Sugarscape (event-driven) case.

Chapter 7

Dependent Types

The pure functional implementation techniques have a number of technical benefits but don't help as much in closing the gap between specification and implementation as one is used from functional programming in general. Therefore we take a step back and abstract from these highly complex implementation techniques and move towards dependent types. Follow [5] and [6].

Conceptually discuss how dependent types can be made of use in ABS without going into lot of technical detail because: 1. i didn't do enough research on it and 2. dependent types seem to be nearly out of focus of the thesis.

Chapter 8

The Gintis Case-Study

Apply my developed techniques to the Gintis paper (and its follow ups: the Ionescu paper [6] and a Masterthesis [14] on it). The aim of this study is to see:

1. Do the techniques transfer to this problem and model?
2. Could pure functional programming have prevented the bugs which Gintis made?
3. Would property-based tests have been of any help to preven the bugs?
4. Could dependent and / or types have prevented the bugs which Gintis made?
5. How close is our (dependently typed) implementation to Ionescus functional specification?
6. When having Cezar Ionescu as external examiner, this chapter will be of great influence as it deals heavily with his work.

Not yet started, need to implement it but there exists code for it already (gintis and java implementations)

8.1 A pure functional implementation

8.2 Exploiting property-based tests

8.3 A dependently typed implementation

8.4 Discussion

Chapter 9

Discussion

This chapter re-visits the aim, objective and hypotheses of the introduction and puts them into perspective with the contributions. Also additional ideas, worth mentioning here (see below) will be discussed here. About 20% exists already.

9.1 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 Agent-Based Simulation. Although we don't have the time to back up our claims with in-depth research, we argue that our findings might be applicable to the following fields at least on a conceptual level.

9.1.1 Simulation in general

We already showed in the paper [35], 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 section ??.

9.1.2 System Dynamics

discuss pure functional system dynamics - correct by construction: benefits: strictly deterministic already at compile time, encode equations directly in code =_i correct by construction. Can serve as backend implementation of visual SD packages.

9.1.3 Discrete Event Simulation

pure functional DES easily possible with my developed synchronous messaging ABS DES in FP: we doing it in gintis study, PDES, should be conceptually easil possible using STM, optimistic approach should be conceptually easier to implement due to persistent data-structures and controlled side-effects

9.1.4 Recursive Simulation

Inspired by [15], add ideas about recursive simulation described in 1st year report and "paper". functional programming maps naturally here due to its inherently recursive nature and controlled side-effects which makes it easier to construct correct recursive simulations. recursive simulation should be conceptually easier to implement and more likely to be correct due to recursive Nature of haskell itself, lack of sideeffects and mutable data

9.1.5 Multi Agent Systems

The fields of Multi Agent Systems (MAS) and ABS are closely related where ABS has drawn much inspiration from MAS [41], [39]. 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 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.

9.2 Peers Framework

TODO: discusses if and how peers object-oriented agent-based modelling framework can be applied to our pure functional approach. TODO: i need to re-read peers framework specifications / paper from the simulation bible book. Although peers framework uses UML and OO techniques to create an agent-based model, we realised from a short case-study with him that most of the framework can be directly applied to our pure functional approach as well, which is not a huge surprise, after all the framework is more a modelling guide than an implementation one. E.g. a class diagram identifies the main datastructures, their operations and relations, which can be expressed equally in our approach - though not that directly as in an oo language but at least the class diagram gives already a good outline and understanding of the required datafields and operations of the respective entities (e.g. agents, environment, actors,...). A state diagram expresses internal states of e.g. an agent, which we discussed

how to do in both our time- and even-driven approach. A sequence diagram e.g. expresses the (synchronous) interactions between agents or with their environment, something for which we developed techniques in our event-driven approach and we discuss in depth there.

Chapter 10

Conclusions

This chapter concludes the whole thesis and outlines future research. Roughly 20% exists already.

10.1 Further Research

1. generalise concepts explored into a pure functional ABS library in Haskell (called chimera),
2. dependent types and linear types are the next big step, towards a stronger formalisation of agents and ABS,
3. find an efficient algorithm for synchronous agent-interactions in concurrent STM ABS

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Appendices

Datasets, lengthy code, additional proofs.