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2ND YEAR REPORT

# Pure Functional Agent-Based Simulation

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June 4, 2018

## Abstract

TODO: we need to distinguish between various meanings of 'correct' 1. correctness of software: the implementation is correct up to a model specification 2. correctness of a simulation: the implementation is correct up to a model specification AND it generates the same dynamics

This Ph.D. investigates how Agent-Based Simulations (ABS) can be implemented using the functional programming paradigm and what the benefits and drawbacks are when doing so. Due to the nature of the functional paradigm we hypothesize that by using this approach we can increase the correctness and gain insights into dynamics of the simulation to on an unprecedented level not possible with the established object-oriented approaches in the field. The correctness of a simulation and its results is of paramount interest in scientific computing thus making our research high impact.

So far we researched *how* to do ABS using the functional paradigm, where we implemented a highly promising approach by building on Functional Reactive Programming using the library Yampa and generalising it to Monadic Stream Functions. By this we could show that ABS is indeed very possible in functional programming as it allowed us to implement a number of different agent-based models, incorporating discrete time-semantics similar to Discrete Event Simulation and continuous time-flows like System Dynamics.

During the research conducted so far, it became apparent that this approach exhibits a few unique properties which indeed supports our initial hypothesis. We have started to systematically explore these properties and will commit our research of the remaining year to develop this fully.

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# Chapter 1

## Introduction

In the first half of the Ph.D. I have investigated *how* to do agent-based simulation in functional programming. This step was necessary because there didn't exist any research, implementation or anything which could be used. Also it served to develop a very deep understanding of functional programming and its combination with agent-based simulation (ABS).

In this process, it became apparent that there are a few unique benefits over the established, state-of-the-art object-oriented approaches which can be subsumed under the common category of *increasing the correctness of the software / simulation*. This insight didn't come as a surprise as this is what the functional programming paradigm is known for and this was also the hypothesis with which we started with: *Functional programming will allow us to write ABS which is more likely to be correct*. Note that, strictly speaking, a software / simulation is either correct or not but we cannot decide this generally for software unless we are willing to pour in an extreme amount of formalisms and tests, so when we say 'increasing the correctness' or 'more likely to be correct' we mean that we can guarantee less bugs and less sources of potential bugs.

We commit the next year of the Ph.D. to explore this insight in a rigorous way and push it to new levels. We hypothesise that this will allow us to write simulations which are *very* likely to be correct and allow a much deeper level of formal and informal reasoning, something not possible with the established object-oriented approaches of the field yet. Because correctness is of paramount importance in scientific computing, our research is a valuable contribution to the field and can be regarded as high impact work.

In the next section of this chapter we will briefly discuss our approach of *how* agent-based simulation can be done with the functional paradigm and its benefits and drawbacks. Then we will give a short overview of *why* this is of benefit and introduce concepts which will outline the research for the next year.

In the following chapters we will give an in-depth introduction to the concepts used in the research of the following year, namely Verification & Validation in Chapter 2 and Dependent Types in Chapter 3. We also have included updated chapters on Aims & Objectives 4, Work to Date 5 and Future Work Plan

6.

## 1.1 The How

The essence of *how* to do agent-based simulation using the functional programming paradigm is described in the paper found in Appendix A. We concluded that the benefits of using the functional programming paradigm as in Haskell has the following benefits in agent-based simulation:

1. Run-Time robustness - restrict the classes of bugs which occur at run-time (we can have run-time bugs in haskell when we are partial!)
2. Compile-Time guarantees - express stronger guarantees already at compile time (TODO: need examples) maybe this is true for Scala as well? but then again, scala is not the traditional approach,
3. Purity: explicit in the types about side-effects and can handle side-effects explicitly in a controlled way - no non-deterministic side-effects, also can control side-effects much better e.g. Random-Numbers and State
4. Explicit Data-Flow: no implicit data-dependencies (if we are excluding IO) - this makes reasoning of data-dependencies and data-flow much easier as compared to traditional oo approaches which utilize pointers or references
5. Declarative: describing WHAT a system is, instead of HOW (imperative) it works - in this way it is much easier to reason about a system and its (expected) behaviour

Despite the benefits we found that agent-agent and agent-environment interactions are very different because method calls and mutable data are not available. While this is the backbone of the advantages, it also is the backbone of the disadvantages: we had to invent new techniques for these kind of interactions which makes functional agent-based simulation conceptually more difficult to understand and implement models with, but it makes those interactions more expressive and explicit and separates them into different categories which are conceptually different but are almost always implemented the same way in object-oriented approaches.

So far, performance is not comparable to object-oriented approaches, but that was not the main focus of the research. Also functional programming as we introduce it to ABS can exploit parallelism nearly for free which should allow speeding up of simulations very easily, and if it is just running multiple replications in parallel. We leave this for further research as investigating this is worth a Ph.D. on its own.

## 1.2 The Why

line of argument 1. established methods need extensive unit-testing for establishing correctness of software, which only increases the likelihood of correctness

and doesn't guarantee it because they are inherent dynamic, testing run-time behaviour, because of the different type system. 2. functional programming as in Haskell has a strong static type system which allows to shift much much more guarantees towards static, compile-time, making many run-time tests obsolete and can guarantee a few things already at compile-time which makes tests to cover that completely obsolete 3. dependent types can push these guarantees even further and theoretically should allow to express guarantees at compile time to an arbitrary complex level which in theory should allow us to abandon run-time testing of bugs altogether. This does not mean that we don't need any tests anymore, as will be outlined in the chapter on Verification & Validation 2. 4. with shifting more towards compile-time guarantees we automatically gain more confidence into the correctness of our simulation and reduce the implementation overhead of writing tests for those cases. Also some properties are simply not testable with run-time tests e.g. that some property holds forever - this is only possible to guarantee by looking at the code directly (where functional programming shines) or expressing it through compile-time guarantees.

The established approach to implement ABS falls into three categories:

1. Programming from scratch using object-oriented languages where Java and Python are 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 one.
3. Using a high-level ABS toolkit for non-programmers, which allow customization through programming. By far the most popular ones is NetLogo with an imperative programming approach followed by AnyLogic with an object-oriented Java approach.

In general one can say that those approaches (especially the 3rd one) support fast prototyping of simulations which allow quick iteration times to explore the dynamics of a model. All of them ultimately suffer from same problems when it comes to verifying the correctness of the implemented simulation. The established way to test software in traditional object-oriented approaches is writing unit-tests which cover all possible cases. This is possible in approach 1 and 2 but very hard or even impossible when using an ABS toolkit as in 3 which is why this approach basically employs manual testing. In general writing those tests or conducting manual tests is necessary because one cannot guarantee the correct working at compile-time which means testing ultimately tests the correct behaviour of code at run-time. The reason why this is not possible is due to the very different type-systems and paradigm of those approaches. Java has a strong but very dynamic type-system whereas Python is completely dynamic not requiring the programmer to put types on data or variables at all - this means that due to type-errors and data-dependencies run-time errors can occur which origins are very difficult to track down.

It is no coincidence that JavaScript, the most widely used language for programming client-side web-applications, originally a completely dynamically

typed language like Python, got additions for type-checking / type-checkers developed by the industry and added a type-system in its last version (TODO cite). This is a sign that the industry acknowledges types as something important as they allow to rule out certain classes of bugs at run-time and express guarantees already at compile-time. We expect similar things to happen with Python as its popularity is surging and more and more people become aware of that problem. Still due to the highly dynamic nature of the type-system, run-time errors are still possible both in Python and Java (and JavaScript).

In general, Types guide us in program construction by restricting the operations we can perform on the data. This means that by choosing types this reveals already a lot of our program and data and prevents us from making mistakes e.g. interpreting some binary data as text instead of a number. In strongly statically typed languages the types can do this already at compile time which allows to rule out certain bugs already at compile time. In general, we can say that for all bugs which can be ruled out at compile time, we don't need to write property- or unit-tests for them, because those bugs cannot - per definition - occur at run-time, so it won't make sense to test their absence at run-time. Also, as Dijkstra famously put it: "Testing shows the presence, not the absence of bugs" - thus by induction we can say that compile time guarantees save us from a potentially infinite amount of testing.

In general it is well established, that pure functional programming as in Haskell, allows to express much stronger guarantees about the correctness of a program *already at compile-time*. This is in fundamental contrast to imperative object-oriented languages like Java or Python where only primitive guarantees about types - mostly relationships between type-hierarchies - can be expressed at compile time which directly implies that one needs to perform much more testing (user testing or unit testing) at *run-time* to check whether the model is sufficiently correct. Thus guaranteeing properties already at compile-time frees us from writing unit tests which cover these cases or test them at run time because they are *guaranteed to be correct under all circumstances, for all inputs*. In this regard we see pure functional programming as truly superior to the traditional object oriented approaches: they lead to implementations of models which are more likely correct because we can express more guarantees already at compile time which directly leads to less bugs which directly increases the probability of the software being a correct implementation of the model.

Having established this was only the first step in our paper in Appendix A. The next step which follows directly, is to move towards dependent types using the language Idris. Generally speaking, dependent types allow to push compile-time guarantees to a new level where we can express nearly arbitrary complex guarantees at compile-time because we can *compute types at compile time*. This means that types are first-class citizen of the language and go as far as being formal proofs of the correctness of an implementation. We hypothesise that the use of dependent types allows us to push the judgement of the correctness of a simulation to new, unprecedented level, not possible with the established object-oriented approaches so far.



## Chapter 2

# Verification & Validation

<http://www2.econ.iastate.edu/tesfatsi/VVAccreditationSimModels.0Balci1998.pdf> : verification = are we building the model right? validation = are we building the right model?

good paper <http://www2.econ.iastate.edu/tesfatsi/VVAccreditationSimModels.0Balci1998.pdf> : very nice 15 guidelines and life cycles, VERY valuable for background and introduction

<http://www2.econ.iastate.edu/tesfatsi/VVSimulationModels.JKleijnen1995.pdf> : suggests good programming practice which is extremely important for high quality code and reduces bugs but real world practice and experience shows that this alone is not enough, even the best programmers make mistakes which often can be prevented through a strong static or a dependent type system already at compile time. What we can guarantee already at compile time, doesn't need to be checked at run-time which saves substantial amount of time as at run-time there may be a huge number of execution paths through the simulation which is almost always simply not feasible to check (note that we also need to check all combinations). This paper also cites modularity as very important for verification: divide and conquer and test all modules separately. this is especially easy in functional programming as composability is much better than with traditional oop due to the lack of interdependence between data and code as in objects and the lack of global mutable state (e.g. class variables or global variables) - this makes code extremely convenient to test. The paper also discusses statistical tests (the t test) to check if the outcome of a simulation is sufficiently close to real-world dynamics. Also the paper suggests using animations to visualise the processes within the simulation for verification purposes (of course they note that animation may be misleading when one focuses on too short simulation runs).

good paper: [https://link.springer.com/chapter/10.1007/978-3-642-01109-2\\_10](https://link.springer.com/chapter/10.1007/978-3-642-01109-2_10) -> verification. "This is essentially the question: does the model do what we think it is supposed to do? Whenever a model has an analytical solution, a condition which embraces almost all conventional economic theory, verification is a matter of checking the mathematics." -> validation: "In an important sense,

the current process of building ABMs is a discovery process, of discovering the types of behavioural rules for agents which appear to be consistent with phenomena we observe.” = „can we encode phenomena we observe in the types? can we use types for the discovery process as well? can dependent types guide our exploratory approach to ABS? - „Because such models are based on simulation, the lack of an analytical solution (in general) means that verification is harder, since there is no single result the model must match. Moreover, testing the range of model outcomes provides a test only in respect to a prior judgment on the plausibility of the potential range of outcomes. In this sense, verification blends into validation.”

either one has an analytical model as the basis of an agent-based model (ABM) or one does not. In the former case, e.g. the SIR model, one can very easily validate the dynamics generated by the ABM to the one generated by the analytical solution (e.g. through System Dynamics). Of course the dynamics won't be exactly the same as ABS discretizes the approach and introduces stochastics which means, one must validate averaged dynamics. In the latter case one has basically no idea or description of the emergent behaviour of the system prior to its execution. It is important to have some hypothesis about the emergent property / dynamics. The question is how verification / validation works in this setting as there is no formal description of the expected behaviour: we don't have a ground-truth against which we can compare our simulation dynamics. (eventuell hilft hier hans vollbrecht weiter: Simulation hat hier den Sinn, die Controller anhand der Roboter Aufgabe zu validieren, Bei solchen Simulationen ist man interessiert an allen möglichen Sequenzen, und da das meist zu viele sind, an einer möglichst gut verteilten Stichprobenmenge. Hier geht es weniger um richtige Zeitmodellierung, sondern um den Test aller möglichen Ereignissequenzen.)

look into DEVS

TODO: the implementation phase is just one stage in a longer process <http://jasss.soc.surrey.ac.uk/12/1/1.html>

WE FOCUS ON VERIFICATION important: we are not concerned here with validating a model with the real world system it simulates. this is an entirely different problem and focuses on the questions if we have built the right model. we are interested here in extremely strong verification: have we built the model right? we are especially interested in to which extent purely and dependently-typed functional programming can support us in this task.

<http://jasss.soc.surrey.ac.uk/8/1/5.html>: "For some time now, Agent Based Modelling has been used to simulate and explore complex systems, which have proved intractable to other modelling approaches such as mathematical modelling. More generally, computer modelling offers a greater flexibility and scope to represent phenomena that do not naturally translate into an analytical framework. Agent Based Models however, by their very nature, require more rigorous programming standards than other computer simulations. This is because researchers are cued to expect the unexpected in the output of their simulations: they are looking for the 'surprise' that shows an interesting emergent effect in the complex system. It is important, then, to be absolutely clear

that the model running in the computer is behaving exactly as specified in the design. It is very easy, in the several thousand lines of code that are involved in programming an Agent Based Model, for bugs to creep in. Unlike mathematical models, where the derivations are open to scrutiny in the publication of the work, the code used for an Agent Based Model is not checked as part of the peer-review process, and there may even be Intellectual Property Rights issues with providing the source code in an accompanying web page.”

<http://jasss.soc.surrey.ac.uk/12/1/1.html>: ”a prerequisite to understanding a simulation is to make sure that there is no significant disparity between what we think the computer code is doing and what is actually doing. One could be tempted to think that, given that the code has been programmed by someone, surely there is always at least one person - the programmer - who knows precisely what the code does. Unfortunately, the truth tends to be quite different, as the leading figures in the field report, including the following: You should assume that, no matter how carefully you have designed and built your simulation, it will contain bugs (code that does something different to what you wanted and expected), ”Achieving internal validity is harder than it might seem. The problem is knowing whether an unexpected result is a reflection of a mistake in the programming, or a surprising consequence of the model itself. [] As is often the case, confirming that the model was correctly programmed was substantially more work than programming the model in the first place. This problem is particularly acute in the case of agent-based simulation. The complex and exploratory nature of most agent-based models implies that, before running a model, there is some uncertainty about what the model will produce. Not knowing a priori what to expect makes it difficult to discern whether an unexpected outcome has been generated as a legitimate result of the assumptions embedded in the model or, on the contrary, it is due to an error or an artefact created in the model design, its implementation, or its execution.”

general requirements to ABS - modelling progress of time (steward robinson simulation book, chapter 2) - modelling variability (steward robinson simulation book, chapter 2) - fixing random number streams to allow simulations to be repeated under same conditions (steward robinson simulation book, chapter 1.3.2 and chapter 2) - only rely on past - $\lambda$  solved with Arrowized FRP - bugs due to implicitly mutable state - $\lambda$  can be ensured by pure functional programming - ruling out external sources of non-determinism / randomness - $\lambda$  can be ensured by pure functional programming - correct interaction protocols - $\lambda$  can be ensured by dependent state machines - deterministic time-delta - $\lambda$  TODO: can we ensure it through dependent-types at type-level? - repeated runs lead to same dynamics - $\lambda$  can be ensured by pure functional programming

steward robinson simulation book bulletpoints - chapter 8.2: speed of coding, transparency, flexibility, run-speed - chapter 8.3: three activities - 1 coding, 2 testing verification and white-box validating, 3 documenting - chapter 9.7: nature of simulation: terminating vs. non-terminating - chapter 9.7: nature of simulation output: transient or steady-state (steady-state cycle, shifting steady-state)

steward robinson simulation book on implementation - meaning of imple-

mentation -¿ 1 implementing the findings: conduct a study which defines and gathers all findings about the model and document them -¿ 2 implementing the model -¿ 3 implementing the learning

steward robinson simulation book on verification, validation and confidence

- Verification is the process of ensuring that the model design has been transformed into a computer model with sufficient accuracy (Davis 1992)
- Validation is the process of ensuring that the model is sufficiently accurate for the purpose at hand (Carson 1986).
- Verification has a narrow definition and can be seen as a subset of the wider issue of validation
- In Verification and validation the aim is to ensure, that the model is sufficiently accurate, which always implies its purpose.
- =¿ the purpose / objectives must be known BEFORE it is validated
- white-box validation: detailed, micro check if each part of the model represent the real world with sufficient accuracy
- ¿ intrinsic to model coding
- black-box validation: overall, macro check whether the model provides a sufficiently accurate representation of the real world system
- ¿ can only be performed once model code is complete
- other definition of verification: it is a test of the fidelity with which the conceptual model is converted into the computer model
- verification (and validation) is a continuous process =¿ if it is already there in the programming language / supported by it e.g. through types,... then this is much easier to do
- difficulties of verification and validation
- ¿ there is no such thing as general validity: a model should be built for one purpose as simple as possible and not be too general, otherwise it becomes too bloated and too difficult / impossible to analyse
- ¿ there may be no real world to compare against: simulations are developed for proposed systems, new production / facilities which dont exist yet.
- ¿ which real world?: the real world can be interpreted in different ways =¿ a model valid to one person may not be valid to another
- ¿ often the real world data are inaccurate
- ¿ there is not enough time to verify and validate everything
- ¿ confidence, not validity: it is not possible to prove that a model is valid, instead one should think of confidence in its validity.
- ¿ verification and validation is thus not the proof that a model is correct but trying to prove that the model is incorrect, the more tests/checks one carries out which show that it is NOT incorrect, the more confidence we can place on the models validity
- methods of verification and validation
- ¿ conceptual model validation: judgment based on the documentation
- ¿ data validation: analysing data for inconsistencies
- ¿ verification and white-box validation
- ¿ both conceptually different but often treated together because both occur continuously through model coding
- ¿ what should be checked: timings (cycle times, arrival times,...), control of elements (breakdown frequency, shift patterns), control flows (e.g. routing), control logic (e.g. scheduling, stock replenishment), distribution sampling (samples obtained from an empirical distribution)
- ¿ verification and white-box validation methods
- ¿ checking code: reading through code and ensure right data and logic is there. explain to others/discuss together/others should look at your code.
- ¿ Visual checks
- ¿ inspecting output reports

- ¿ black-box testing: consider overall behaviour of the model without looking into its parts, basically two ways
- ¿ comparison with the real system: statistical tests
- ¿ comparison with another model (e.g. mathematical equations): could

compare exactly or also through statistical tests -;

peers slides: - Model testing (verification and validation) -; Required to place confidence in a study's results -; Model testing is not a process of trying to demonstrate that the model is correct but a process of trying to prove that the model is incorrect!

- Model verification: The process of ensuring that the model design has been transformed into a computer model with sufficient accuracy - Model validation: The process of ensuring that the model is sufficiently accurate for the purpose at hand -; models are not meant to be completely accurate -; models are supposed to be build for a specific purpose

- Data Validation: Determining that the contextual data and the data required for model realisation and validation are sufficiently accurate for the purpose at hand.

- white-Box Validation: Determining that the constituent parts of the computer model represent the corresponding real world elements with sufficient accuracy for the purpose at hand (micro check) -; how: Checking the code, visual checks, inspecting output reports

- Black-Box Validation: Determining that the overall model represents the real world with sufficient accuracy for the purpose at hand (macro check) -; comparison with the real system -; comparison with other (simpler) models

- Experimentation Validation: Determining that the experimental procedures adopted are providing results that are sufficiently accurate for the purpose at hand. -; How can we do this? - Graphical or statistical methods for determining warm-up period, run length and replications (to obtain accurate results) - Sensitivity analysis (to improve the understanding of the model)

- Solution Validation: Determining that the results obtained from the model of the proposed solution are sufficiently accurate for the purpose at hand -; How does this differ from Black Box Validation? Solution validation compares the model of the proposed solution to the implemented solution while black-box validation compares the base model to the real world -; How can we do this? Once implemented it should be possible to validate the implemented solution against the model results

- Verification: Testing the fidelity with which the conceptual model is converted into the computer model. Verification is done to ensure that the model is programmed correctly, the algorithms have been implemented properly, and the model does not contain errors, oversights, or bugs.

-; How can we do this? Same methods as for white-box validation (checking the code, visual checks, inspecting output reports) but ... Verification compares the content of the model to the conceptual model while white-box validation compares the content of the model to the real world

- Difficulties of verification and validation -; There is no such thing as general validity: a model is only valid with respect to its purpose -; There may be no real world to compare against -; Which real world? Different people have different interpretations of the real world -; Often real world data are inaccurate: If the data are not accurate it is difficult to determine if the model's results are correct. Even if the data is accurate, the real world data are only a sample, which in

itself creates inaccuracy - There is not enough time to verify and validate every aspect of a model

- Some final remarks: V&V is a continuous and iterative process that is performed throughout the life cycle of a simulation study. Example: If the conceptual model is revised as the project progresses it needs to be re-validated - V&V work together by removing barriers and objections to model use and hence establishing credibility.

- Conclusion: Although, in theory, a model is either valid or not, proving this in practice is a very different matter. It is better to think in terms of confidence that can be placed in a model!

### 2.0.1 Testing

TODO: explore ABS testing in pure functional Haskell - we need to distinguish between two types of testing/verification 1. testing/verification of models for which we have real-world data or an analytical solution which can act as a ground-truth. examples for such models are the SIR model, stock-market simulations, social simulations of all kind 2. testing/verification of models which are just exploratory and which are only be inspired by real-world phenomena. examples for such models are Epsteins Sugarscape and Agent Zero

### 2.0.2 Black Box Verification

Defined as treating the functionality to test as a black box with inputs and outputs and comparing controlled inputs to expected outputs.

In Black Box Verification one generally feeds input and compares it to expected output. In the case of ABS we have two things to black-box test:

1. Isolated Agent Behaviour - test isolated agent behaviour under given inputs using unit- and property-based testing
2. Interacting Agent Behaviour - test if interaction between agents are correct
3. Simulation Dynamics - compare emergent dynamics of the ABS as a whole under given inputs to an analytical solution / real-world dynamics in case there exists some using statistical tests
4. Hypotheses- test whether hypotheses are valid / invalid using unit- and property-based testing. TODO: how can we formulate hypotheses in unit- and/or property-based tests?

- testing of the final dynamics: how close do they match the analytical solution - can we express model properties in tests e.g. quickcheck? - property-testing shines here - isolated tests: how easy can we test parts of an agent / simulation?

### 2.0.2.1 Finding optimal $\Delta t$

The selection of the right  $\Delta t$  can be quite difficult in FRP because we have to make assumptions about the system a priori. One could just play it safe with a very conservatively selected small  $\Delta t \leq 0.1$  but the smaller  $\Delta t$ , the lower the performance as it quickly multiplies the number of steps to calculate. Obviously one wants to select the *optimal*  $\Delta t$ , which in the case of ABS is the largest possible  $\Delta t$  for which we still get the correct simulation dynamics. To find out the *optimal*  $\Delta t$  one can make direct use of the Black Box tests: start with a large  $\Delta t = 1.0$  and reduce it by half every time the tests fail until no more tests fail - if for  $\Delta t = 1.0$  tests already pass, increasing it may be an option. It is important to note that although isolated agent behaviour tests might result in larger  $\Delta t$ , in the end when they are run in the aggregate system, one needs to sample the whole system with the smallest  $\Delta t$  found amongst all tests. Another option would be to apply super-sampling to just the parts which need a very small  $\Delta t$  but this is out of scope of this paper.

### 2.0.2.2 Agents as signals

Agents *might* behave as signals in FRP which means that their behaviour is completely determined by the passing of time: they only change when time changes thus if they are a signal they should stay constant if time stays constant. This means that they should not change in case one is sampling the system with  $\Delta t = 0$ . Of course to prove whether this will *always* be the case is strictly speaking impossible with a Black Box verification but we can gain a good level of confidence with them also because we are staying pure. It is only through white box verification that we can really guarantee and prove this property.

### 2.0.2.3 Comparison of dynamics against existing data

- utilise a statistical test with H0 "ABS and comparison is not the same" and H1 "ABS and comparison is the same" - how many replications and how do we average? - which statistical test do we implement? (steward robinson simulation book, chapter 12.4.4) - Normalized Mean Squared Error (NMSE) - TODO: implement confidence interval - TODO: what about chi-squared? - TODO: what about paired-t confidence interval

IMPORTANT: this is not what we are after here in this paper, statistical tests are a science on their own and there actually exists quite a large amount of literature for conducting statistical tests on ABS dynamics: Robinson Book (TODO: find additional literature)

## 2.0.3 White Box Verification

White-Box verification is necessary when we need to reason about properties like *forever*, *never*, which cannot be guaranteed from black-box tests. Additional help can be coverage tests with which we can show that all code paths have been covered in our tests.

# Chapter 3

## Dependent Types

### 3.0.1 Dependent Types

We see this paper 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 [16, 11, 1].

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 [4] 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 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:

- Accessing the environment in section ?? involves indexed array access which is always potentially dangerous as the indices have to be checked at run-time.

Using dependent types it should be possible to encode the environment dimensions into the types. In combination with suitable data types for coordinates one should be able to ensure already at compile time that access happens only within the bounds of the environment.

- In the SIR implementation one could make wrong state-transitions e.g.



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 many agent-based models define their agents in terms of state-machines.

- An infected agent recovers after a given time - the transition of infected to recovered is a timed transition. Nothing prevents us from *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.

- 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 our implementation, we terminate the SIR model always after a fixed number of time-steps. We can informally reason that restricting the simulation to a fixed number of time-steps is not necessary because the SIR model *has to* reach a steady state after a finite number of steps. This means that at that point the dynamics won't change any more, thus one can safely terminate the simulation. Informally speaking, the reason for that is that eventually the system will run out of infected agents, which are the drivers of the dynamic. We know that all infected agents will recover after a finite number of time-steps *and* that there is only a finite source for infected agents which is monotonously decreasing.

Using dependent types it might be possible to encode this in the types, resulting 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.

TODO: give a more in-depth explanation of dependent types:

- dependently typed functions (pi types) - dependent pairs (sigma types) - equality types - type-level computations - totality

dependent types: model- vs. agent-centric. model-centric means one looks at the model and its specifications as a whole and encodes them e.g. totality of

SIR. agent-centric means one looks only at the agent level and encodes that as dependently typed as possible and hopes that model guarantees emerge: emergence on a metalevel - put otherwise: does the totality of SIR emerge when we follow an agent-centric approach?

Independent of the programming paradigm, there exist fundamentally two approaches implementing agent-based simulation: time- and event-driven. In the time-driven approach, the simulation is stepped in fixed  $\Delta t$  and all agents are executed at each time-step - they act virtually in lock-step at the same time. The approach is inspired by the theory of continuous system dynamics (TODO: cite). In the event-driven approach, the system is advanced through events, generated by the agents, and the global system state changes by jumping from event to event, where the state is held constant in between. The approach is inspired by discrete event simulation (DES) (TODO: citation) which is formalized in the DEVS formalism [18].

In a preceding paper we investigated how to derive a time-driven pure functional ABS approach in Haskell (TODO: cite my paper). We came to quite satisfactory results and implemented also a number of agent-based models of various complexity (TODO: cite schelling, sugarscape, agent zero). Still we identified weaknesses due to the underlying functional reactive programming (FRP) approach. It is possible to define partial implementations which diverge during runtime, which may be difficult to determine for complex models for a programmer at compile time. Also sampling the system with fixed  $\Delta t$  can lead to severe performance problems when small  $\Delta t$  are required, as was shown in our paper. The later problem is well known in the simulation community and thus as a remedy an event-driven approach was suggested [12]. In this paper for the first time, we derive a pure functional event-driven agent-based simulation. Instead of using Haskell, which provides already libraries for DES [15], we focus on the dependently typed pure functional programming language Idris. In our previous paper we hypothesised that dependent types may offer interesting new insights and approaches to ABS but it was unclear how exactly we can make use of them, which was left for further research. In this paper we hypothesise that, as opposed to a time-driven approach, the event-driven approach is especially suited to make proper use of dependent types due to its different nature. Note that both a pure functional event-driven approach to ABS *and* the use of dependent types in ABS has so far never been investigated, which is the unique contribution of this paper. If we can construct a dependently typed program of the SIR ABM which is total, then we have a proof-by-construction that the SIR model reaches a steady-state after finite time

Dependent Types are the holy grail in functional programming as they allow to express even stronger guarantees about the correctness of programs and go as far where programs and types become constructive proofs [17] which must be total by definition [16], [2], [?], [13]. Thus the next obvious step is to apply them to our pure functional approach of agent-based simulation. So far no research in applying dependent types to agent-based simulation exists at all and it is not clear whether dependent types do make sense in this setting. We 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. Note that we can only scratch the surface and lay down basic ideas and leave a proper in-depth treatment of this topic for further research. We use Idris [4], [7] as 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 promise the following:

1. Types as proofs - In dependently types languages, types can depend on any values and are first-class objects themselves. TODO: make more clear
2. Totality and termination - Constructive proofs 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. A total function is defined by [7] as: it terminates with a well-typed result or produces a non-empty finite prefix of a well-typed infinite result in finite time. Idris is turing complete but is able to check the totality of a function under some circumstances but not in general as it would imply that it can solve the halting problem. Other dependently typed languages like Agda or Coq restrict recursion to ensure totality of all their functions - this makes them non turing complete.

dependent-types: - $\lambda$  encode model-invariants on a meta-level - $\lambda$  encode dynamics (what? feedbacks? positive/negative) on a meta-level - $\lambda$  totality equals steady-state of a simulation, can enforce totality if required through type-level programming - $\lambda$  probabilistic types can encode probability distributions in types already about which we can then reason - $\lambda$  can we encode objectives in types? - $\lambda$  agents as dependently typed continuations?: need a dependently typed concept of a process over time

### 3.0.2 Related Work

The authors of [3] 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.

The authors of [8] use depend types to implement correct-by-construction concurrency in the Idris language [4]. They introduce the concept of a Embedded Domain Specific Language (EDSL) for concurrently locking/unlocking and

reading/writing of resources and show that an implementation and formalisation are the same thing when using dependent types. We can draw inspiration from it by taking into consideration that we might develop a EDSL in a similar fashion for specifying general commands which agents can execute. The interpreter of such a EDSL can be pure itself and doesn't have to run in the IO Monad as our previous research (TODO: cite my PFE paper) has shown that ABS can be implemented pure.

In [9] the authors discuss systems programming with focus on network packet parsing with full dependent types in the Idris language [4]. Although they use an older version of it where a few features are now deprecated, they follow the same approach as in the previous paper of constructing an EDSL and writing an interpreter for the EDSL. In a longer introduction of Idris the authors discuss its ability for termination checking in case that recursive calls have an argument which is structurally smaller than the input argument in the same position and that these arguments belong to a strictly positive data type. We are particularly interested in whether we can implement an agent-based simulation which termination can be checked at compile time - it is total.

In [5] the author discusses programming and reasoning with algebraic effects and dependent types in the Idris language [4]. They claim that monads do not compose very well as monad transformer can quickly become unwieldy when there are lots of effects to manage. As a remedy they propose algebraic effects and implement them in Idris and show how dependent types can be used to reason about states in effectful programs. In our previous research (TODO: cite my PFE paper) we relied heavily on Monads and transformer stacks and we indeed also experienced the difficulty when using them. Algebraic effects might be a promising alternative for handling state as the global environment in which the agents live or threading of random-numbers through the simulation which is of fundamental importance in ABS. Unfortunately algebraic effects cannot express continuations (according to the authors of the paper) which is but of fundamental importance for pure functional ABS as agents are on the lowest level built on continuations - synchronous agent interactions and time-stepping builds directly on continuations. Thus we need to find a different representation of agents - GADTs seem to be a natural choice as all examples build heavily on them and they are very flexible.

In [10] the authors apply dependent types to achieve safe and secure web programming. This paper shows how to implement dependent effects, which we might draw inspiration from of how to implement agent-interactions which, depending on their kind, are effectful e.g. agent-transactions or events.

In [6] the author introduces the ST library in Idris, which allows a new way of implementing dependently typed state machines and compose them vertically (implementing a state machine in terms of others) and horizontally (using multiple state machines within a function). In addition this approach allows to manage stateful resources e.g. create new ones, delete existing ones. We can draw further inspiration from that approach on how to implement dependently typed state machines, especially composing them hierarchically, which is a common use case in agent-based models where agents behaviour is mod-

elled through hierarchical state-machines. As with the Algebraic Effects, this approach doesn't support continuations (TODO: is this so?), so it is not really an option to build our architecture for our agents on it, but it may be used internally to implement agents or other parts of the system. What we definitely can draw inspiration from is the implementation of the indexed Monad *STrans* which is the main building block for the ST library.

The book [7] is a great source to learn pure functional dependently typed programming and in the advanced chapters introduces the fundamental concepts of dependent state machine and dependently typed concurrent programming on a simpler level than the papers above. One chapter discusses on how to implement a messaging protocol for concurrent programming, something we can draw inspiration from for implementing our synchronous agent interaction protocols.

The authors of [14] apply dependent types to FRP to avoid some run-time errors and implement a dependently typed version of the Yampa library in Agda. FRP was the underlying concept of implementing agent-based model we took on in our previous approach (TODO: cite). We could have taken the same route and lift FRP into dependent types but we chose explicitly to not go into this direction and look into complementing approaches on how to implement agent-based models.

The fundamental difference to all these real-world examples is that in our approach, the system evolves over time and agents act over time. A fundamental question will be how we encode the monotonous increasing flow of time in types and how we can reflect in the types that agents act over time.

### 3.1 Concepts of Dependent Types in Agent-Based Simulation

Independent of the programming paradigm, there exist fundamentally two approaches implementing agent-based simulation: time- and event-driven. In the time-driven approach, the simulation is stepped in fixed  $\Delta t$  and all agents are executed at each time-step - they act virtually in lock-step at the same time. The approach is inspired by the theory of continuous system dynamics (TODO: cite). In the event-driven approach, the system is advanced through events, generated by the agents, and the global system state changes by jumping from event to event, where the state is held constant in between. The approach is inspired by discrete event simulation (DES) (TODO: citation) which is formalized in the DEVS formalism [18].

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during runtime, which may be difficult to determine for complex models for a programmer at compile time. Also sampling the system with fixed  $\Delta t$  can lead to severe performance problems when small  $\Delta t$  are required, as was shown in our paper. The later problem is well known in the simulation community and thus as a remedy an event-driven approach was suggested [12]. In this paper for the first time, we derive a pure functional event-driven agent-based simulation. Instead of using Haskell, which provides already libraries for DES [15], we focus on the dependently typed pure functional programming language Idris. In our previous paper we hypothesised that dependent types may offer interesting new insights and approaches to ABS but it was unclear how exactly we can make use of them, which was left for further research. In this paper we hypothesise that, as opposed to a time-driven approach, the even-driven approach is especially suited to make proper use of dependent types due to its different nature. Note that both a pure functional event-driven approach to ABS *and* the use of dependent types in ABS has so far never been investigated, which is the unique contribution of this paper. If we can construct a dependently typed program of the SIR ABM which is total, then we have a proof-by-construction that the SIR model reaches a steady-state after finite time

Dependent Types are the holy grail in functional programming as they allow to express even stronger guarantees about the correctness of programs and go as far where programs and types become constructive proofs [17] which must be total by definition [16], [2], [?], [13]. Thus the next obvious step is to apply them to our pure functional approach of agent-based simulation. So far no research in applying dependent types to agent-based simulation exists at all and it is not clear whether dependent types do make sense in this setting. We 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. Note that we can only scratch the surface and lay down basic ideas and leave a proper in-depth treatment of this topic for further research. We use Idris [4], [7] as 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.

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Coq restrict recursion to ensure totality of all their functions - this makes them non turing complete.

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As shown in our previous research (TODO: cite), the strong static type system of Haskell allows us to guarantee a lot already at compile time:

- Purity - no side-effects possible at all
- Monad - controlled, explicit side-effects possible
- generic types allow to guarantee for all

Dependent Types in Idris bring the strong static type system of Haskell to a new level, which allows us to both guarantee more things at compile time and express things through type-level computations. This means the following at compile time

- Ruling out ever larger classes of bugs
- Dependent State Machines
- Dependent Agent Interactions
- Flow Of Time
- Totality
- Constructive Proofs

### 3.1.1 Ruling out Bugs

1. Index out of bounds access of Lists and Vectors can be guaranteed not to happen any more when using proofs of existence of the element in the list or vector.
2. Size of list or vector stays constant / increases / decreases / sum of length of multiple vectors guaranteed to be of some number

The question is how far we can generalise our approaches because we fear that the downside of using dependently typed abs is that every implementation needs to start from Scratch: we cant write a general library for it like chimera because the more we put into types, the more specific it is = $\lambda$  individual implementation which reuses existing 'patterns' like state machines, messages,...

### 3.1.2 General Agent Interface

using dependent types to specify the general commands available for an agent. here we can follow the approach of an DSEL as described in [8] and write then an interpreter for it. It is of importance that the interpreter shall be pure itself and does not make use of any fancy IO stuff.

### 3.1.3 Dependent State Machines

dependent state machines in abs for internal state because that is very Common in ABS. Here we can draw inspiration from the paper [6] and book [7].

### 3.1.4 Environment

One of the main advantages of Agent-Based Simulation over other simulation methods e.g. System Dynamics is that agents can live within an environment. Many agent-based models place their agents within a 2D discrete NxM environment where agents either stay always on the same cell or can move freely within the environment where a cell has 0, 1 or many occupants. Ultimately this boils down to accessing a NxM matrix represented by arrays or a similar data structure. In imperative languages accessing memory always implies the danger of out-of-bounds exceptions *at run-time*. With dependent types we can represent such a 2d environment using vectors which carry their length in the type (TODO: discuss them in background) thus fixing the dimensions of such a 2D discrete environment in the types. This means that there is no need to drag those bounds around explicitly as data. Also by using dependent types like Fin which depend on the dimensions we can enforce at compile time that we can only access the data structure within bounds. If we want to we can also enforce in the types that the environment will never be an empty one where  $N, M \geq 0$ .

```

Disc2dEnv : (w : Nat) -> (h : Nat) -> (e : Type) -> Type
Disc2dEnv w h e = Vect (S w) (Vect (S h) e)

data Disc2dCoords : (w : Nat) -> (h : Nat) -> Type where
  MkDisc2dCoords : Fin (S w) -> Fin (S h) -> Disc2dCoords w h

centreCoords : Disc2dEnv w h e -> Disc2dCoords w h
centreCoords {w} {h} _ =
  let x = halfNatToFin w
      y = halfNatToFin h
  in mkDisc2dCoords x y
where
  halfNatToFin : (x : Nat) -> Fin (S x)
  halfNatToFin x =
    let xh = divNatNZ x 2 SIsNotZ
        mfin = natToFin xh (S x)
    in fromMaybe FZ mfin

```



```

setCell : Disc2dCoords w h
         -> (elem : e)
         -> Disc2dEnv w h e
         -> Disc2dEnv w h e
setCell (MkDisc2dCoords colIdx rowIdx) elem env
       = updateAt colIdx (\col => updateAt rowIdx (const elem) col) env

getCell : Disc2dCoords w h
         -> Disc2dEnv w h e
         -> e
getCell (MkDisc2dCoords colIdx rowIdx) env
       = index rowIdx (index colIdx env)

neumann : Vect 4 (Integer, Integer)
neumann = [
            (0, 1),
            (-1, 0), (1, 0),
            (0, -1)]

moore : Vect 8 (Integer, Integer)
moore = [(-1, 1), (0, 1), (1, 1),
         (-1, 0), (1, 0),
         (-1, -1), (0, -1), (1, -1)]

-- TODO: can we express that n <= len?
filterNeighbourhood : Disc2dCoords w h
                   -> Vect len (Integer, Integer)
                   -> Disc2dEnv w h e
                   -> (n ** Vect n (Disc2dCoords w h, e))
filterNeighbourhood {w} {h} (MkDisc2dCoords x y) ns env =
  let xi = finToInteger x
      yi = finToInteger y
  in filterNeighbourhood' xi yi ns env
where
  filterNeighbourhood' : (xi : Integer)
                      -> (yi : Integer)
                      -> Vect len (Integer, Integer)
                      -> Disc2dEnv w h e
                      -> (n ** Vect n (Disc2dCoords w h, e))
  filterNeighbourhood' _ _ [] env = (0 ** [])
  filterNeighbourhood' xi yi ((xDelta, yDelta) :: cs) env
    = let xd = xi - xDelta
        yd = yi - yDelta
        mx = integerToFin xd (S w)
        my = integerToFin yd (S h)
    in case mx of

```

```

Nothing => filterNeighbourhood' xi yi cs env
Just x  => (case my of
  Nothing => filterNeighbourhood' xi yi cs env
  Just y  => let coord      = MkDisc2dCoords x y
              c            = getCell coord env
              (_ ** ret) = filterNeighbourhood' xi yi cs env
              in (_ ** ((coord, c) :: ret)))

```

### 3.1.5 Dependent Agent Interactions

#### 3.1.5.1 Agent Transactions

dependently typed message protocols in ABS because its very common, and easily done thorough methods in OOP: sugarscape mating and trading protocol using a DSEL [8] to restrict the available primitives in the message protocol?

#### 3.1.5.2 Data Flow

TODO: can dependent types be used in the Data Flow Mechanism?

#### 3.1.5.3 Event Scheduling

TODO: can dependent types be used in the event-scheduling mechanism?

### 3.1.6 Flow Of Time

TODO: can dependent types be used to express the flow of time and its strongly monotonic increasing?

### 3.1.7 Totality

totality of parts or the whole simulation e.g. in case of the SIR model we can informally reason that the simulation **MUST** reach an equilibrium (a steady state from which there is no escape: the dynamics won't change anymore, derivations are 0) after a finite number of steps. if we can construct a total program which expresses this, we have a formal proof of that which is 1) a specification of the model 2) generates the dynamics 3) is a proof that it reaches equilibrium

### 3.1.8 Constructive Proofs

- An agent-based model and the simulated dynamics of it is itself a constructive proof which explain a real-world phenomenon sufficiently good - proof of the existence of an agent: holds always only for the current time-step or for all time, depending on the model. e.g. in the SIR model no agents are removed from / added to the system thus a proof holds for all time. In sugarscape agents are removed / added dynamically so a proof might become invalid after a time

or one can construct a proof only from a given time on e.g. when one wants to prove that agent X exists but agent X is only created at time t then before time t the prove cannot be constructed and is uninhabited and only inhabited from time t on.

## 3.2 Dependently Typed SIR

Intuitively, based upon our model and the equations we can argue that the SIR model enters a steady state as soon as there are no more infected agents. Thus we can informally argue that a SIR model must always terminate as:

1. Only infected agents can infect susceptible agents.
2. Eventually after a finite time every infected agent will recover.
3. There is no way to move from the consuming *recovered* state back into the *infected* or *susceptible* state <sup>1</sup>.

Thus a SIR model must enter a steady state after finite steps / in finite time.

This result gives us the confidence, that the agent-based approach will terminate, given it is really a correct implementation of the SD model. Still this does not proof that the agent-based approach itself will terminate and so far no proof of the totality of it was given. 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 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. We hypothesize that it should be possible due to the nature of the state transitions where there are no cycles and that all infected agents will eventually reach the recovered state. Abandoning the FRP approach and starting fresh, the question is how we implement a *total* agent-based SIR model in Idris. Note that in the SIR model an agent is in the end just a state-machine thus the model consists of communicating / interacting state-machines. In the book [7] the author discusses using dependent types for implementing type-safe state-machines, so we investigate if and how we can apply this to our model. We face the following questions: how can we be total? can we even be total when drawing random-numbers? Also a fundamental question we need to solve then is how we represent time: can we get both the time-semantics of the FRP approach of Haskell AND the type-dependent expressivity or will there be a trade-off between the two?

– TODO: express in the types – SUSCEPTIBLE: MAY become infected when making contact with another agent – INFECTED: WILL recover after a finite number of time-steps – RECOVERED: STAYS recovered all the time

---

<sup>1</sup>There exists an extended SIR model, called SIRS which adds a cycle to the state-machine by introducing a transition from recovered to susceptible but we don't consider that here.

– SIMULATION: advanced in steps, time represented as  $\text{Nat}$ , as real numbers are not constructive and we want to be total – terminates when there are no more INFECTED agents

show formally that abs does resemble the sd approach: need an idea of a proof and then implement it in dependent types: look at 3 agent system: 2 susceptible, 1 infected. or maybe 2 agents only

### 3.2.1 A constructive proof of totality

The idea is 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). The dynamics of the system-dynamics SIR model are in equilibrium (won't change anymore) when the infected stock is 0. This can (probably) be shown formally but intuitionistic it 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. 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 need to 'tell' the type-checker the following: 1) no more infected agents is the termination criterion 2) all infected agents will recover after a finite number of time  $=_{\lambda}$  the simulation will eventually run out of infected agents But when we look at the SIR+S model we have the same termination criterion, but we cannot guarantee that it will run out of infected  $=_{\lambda}$  we need additional criteria 3) infected agents are 'generated' by susceptible agents 4) susceptible agents are NOT INCREASING (e.g. recovered agents do NOT turn back into susceptibles) Interesting: can we adopt our solution (if we find it), into a SIRS implementation? this should then break totality. also how difficult is it?

The HOTT book states that lists, trees,... are inductive types/inductively defined structures where each of them is characterized by a corresponding "induction principle". For a proof of totality of SIR we need to find the "induction principle" of the SIR model and implement it. What is the inductive, defining structure of the SIR model? is it a tree where a path through the tree is one simulation dynamics? 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?

TODO: <https://stackoverflow.com/questions/19642921/assisting-agdas-termination-checker/39591118>

## 3.3 Constructivism

TODO: ABS is constructive: "if you can't grow it, you can't explain it" (epstein)  
 TODO: Dependent Types are constructive  $=_{\lambda}$  there are no excluded middle in both approaches  $=_{\lambda}$  are there deeper, philosophical connections going on? does it have even deeper implications? TODO: shortly discuss Propositions

as types from HOTT 1.11. In the end a dependently typed ABS is then a constructive proof of WHAT? the model? if we have a total SIR implementation its a constructive proof that the agent-based implementation is total / will reach an equilibrium after a finite number of steps. Still it is not entirely clear WHAT WE ARE PROVING when we are constructing dependently typed agent-based simulations. I need to think about this more carefully TODO: checkout my notes in 1st annual review on constructivism / popper

Law of excluded middle does not hold anymore because it 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.

An important concept of this constructive approach is that the (proposition of) equality between two elements of the same type are is itself a type, called equality or identity types. This is much more expressive than a boolean proposition which evaluates to True in case they are the same and False if not as an equality type encodes much richer information which can be used by the type system. With the boolean approach, also known as boolean blindness, although one has compare two elements on equality and this check has returned true, the compiler has still no way of knowing *after* the check that both elements are indeed the same - with equality types we can provide this information which can be used by the compiler (TODO: discuss further how this can be of use). If we have an element of this type (speak a witness / the type is inhabited) then we know the two elements are equal.

[16] discusses constructive vs. classic mathematics in chapter 3. In general there are two conflicting philosophical views of the foundations of mathematics: the constructive and the classic one. The constructive view has been identified with realism, empirical computational content where the classical one with idealism and pragmatic. TODO: work through chapter 3

dependent types as a perfect match and correspondence to the constructive nature of ABS, which is a 3rd way after induction and deduction

## 3.4 Foundations

TODO: shortly discuss that dependent types are based on martin-lf intuitions type theory.

### 3.4.1 Intensionality vs. Extensionality

HOTT book, NOTES on chapter 1: "Extensional theory makes no distinction between judgmental and propositional equality, the intensional theory regards judgmental equality as purely definitional, and admits a much broader proof-relevant interpretation of the identity type that is central to the homotopy interpretation."

Propositional equality allows to assume that a variable  $x$  of type  $p$  is equal to  $y$ :  $p : x = y$ .

Judgemental equality (or definitional equality) means "equal by definition" e.g. if we have a function  $f : N \rightarrow N$  by  $f(x) = x^2$  then  $f(3)$  is equal to  $3^2$  by definition. Whether or not two expressions are equal by definition is just a matter of expanding out the definitions, in particular it is algorithmically decidable.

Fact: Idris, Agda and Coq are intensional

## Chapter 4

# Aims and Objectives

TODO: refine and adapt to 2nd year

This chapter gives a compact and concise overview of the aims and objectives. Chapter 6 gives a more in-depth plan and details in how we will approach the aim in general and the objectives in particular.

### 4.1 Aim

The aim of this Ph.D. is to investigate how the pure functional programming paradigm can be used to increase the robustness and gain insights into dynamics of Agent-Based Simulations.

#### 4.1.1 Hypothesis

We claim that using pure functional programming and dependent types in agent-based simulation leads to simulation software which is more likely to be correct, has less sources of bugs and is easier to verify and validate.

### 4.2 Objectives

1. Develop a library for general-purpose Agent-Based Simulation in Haskell to have a tool in the pure functional programming paradigm to be used for conducting the research.
2. Compare the general approach of pure functional programming in the instance of Haskell and object-oriented programming in the instance of Java to implement ABS. Look into differences and similarities and identify benefits and drawbacks.
3. Explore how pure functional programming can increase testability, verification and correctness of Agent-Based Simulations.

4. Investigate to which extent one can use reasoning-techniques of the pure functional paradigm to reason about dynamics in ABS.



## Chapter 5

# Work To Date

From a very general perspective I am researching a novel implementation approach to ABS. The hypothesis is that due to its underlying foundations of pure functional programming, this approach leads to simulation software which is easier to verify and validate and thus more likely to be correct, less sources of bugs and is conceptually cleaner. In the first half of my PhD (October 2016 - March 2018) I have learned the underlying foundations of pure functional programming, did lots of prototyping and ultimately developed a way of implementing ABS in this approach. This resulted in a paper, submitted in March 2018 to the Haskell Symposium 2018, which discusses *how* to do agent-based simulation with pure functional programming as foundation and how to solve the fundamental problems of encapsulating agent-state, doing agent-interactions and bringing in environments in this setting. We found out that we immediately benefit from this approach in various ways, supporting our initial hypothesis but didn't investigate it in scientific details, which we leave for the next 12 months, conducted between April 2018 and April 2019. Thus we will be researching the *why* of our approach, which we claim is an easier and stronger approach to verification and validation (V & V). We need to clarify the meaning of V & V in both areas we trying to gap, pure functional programming and agent-based simulation, and how they related to each other and how we can connect them. Further we need to quantify our claims of less sources of bugs through other research and comparing it to imperative OO approaches. In this time we will investigate the use of dependent types in our pure functional approach to agent-based simulation which we hypothesise should allow an unprecedented level of verification and validation, not possible (even not on a theoretical level) with imperative, traditional object-oriented approaches. There exists literally no research on this topic thus it will form the unique and sufficiently advanced, novel contribution of our PhD to the field. We will also write an additional paper which will investigate how dependent types can be made of use in ABS. Around December 2018 I will start writing another paper which is targeted for an agent-based simulation journal and is written as a conceptual paper, describing the approach and benefits of purely and dependently typed agent-based simulation.

While writing this paper I will start constructing the main argument structure of my thesis so I have structure already when I start writing the thesis in April 2019. The last 6 months of the PhD (April 2019 - September 2019) will be dedicated to writing up the thesis and conducting additional research if still necessary.

So roughly the PhD can be split into 3 phases: Researching the HOW: September 2016 - March 2018 Researching the WHY: April 2018 - March 2019 Writing the Thesis: April 2019 - September 2019

2016 October - December proper learning haskell programming experiments with scala & akka (actor model)

2017 January - March writing 1st paper: Art Of Iteration MGS2017 deepening haskell programming skills

April - July getting into functional reactive programming literature research & 1st year report and review prototyping concepts of purely functional ABS presentation to FP group at FP lunch

August holiday reading book and papers on functional programming

September preparation for social simulation conference 2017 (SSC2017)

October - December working on 2nd paper (pure functional epidemics): first draft generalising the functional reactive programming approach to monadic stream functions

2018 January - February prototyping event-scheduling concepts in pure functional ABS completely reworking 2nd paper: 2nd draft learning Idris language (pure functional, dependently typed programming)

March finalising 2nd paper and submission to Haskell Symposium 2018 deepening Idris knowledge and experience

April bit of work on verification and validation of the purely functional SIR abs implementation using quickcheck. this is not original research but will then be useful for the final thesis as a small separate section started 3rd paper on dependent types in purely functional ABS

May feedback on 2nd paper on 18 May researching concepts of dependent types in purely functional ABS research & writing 3rd paper

June - July 2nd year report & review research & writing 3rd paper

Here we give a concise overview over the activities performed in the 2nd year.

## 5.1 Social Simulation Conference 2017

## 5.2 Paper Published

TODO: Art of Iteration was published in SSC2017 proceedings

## 5.3 Papers Submitted

### 5.3.1 Pure Functional Epidemics

This paper, which is attached in Appendix A

## 5.4 Reports

### 5.4.1 Haskell Communities and Activities Report (HCAR) May 2017

We wrote a new entry for the HCAR May 2017, which tries to compile and publish novel and on-going ideas in the Haskell community. It is freely available under <https://www.haskell.org/communities/05-2017/html/report.html>. We hope that our idea and the work of our PhD gets a bit more attention and may start some discussions with people interested in this work.

### 5.4.2 2nd Year Report

This document.

## 5.5 Talks

So far only two talks were given. The first one was a presentation of the ideas underlying the update-strategies paper at the IMA - seminar day. The second was presenting my ideas about functional reactive ABS to the FP-Lab Group at the FPLunch.

## Chapter 6

# Future Work Plan

2018 August - September research & writing 3rd paper holiday

October - December finalising research & writing 3rd paper

2019 January - April finalising and submitting 3rd paper writing 4th paper: towards pure functional ABS. targeted for an agent-based simulation audience and written as a journal paper. this wont need any unique research but is basically a conceptual paper explaining my insights and research so far on a not too technical level to the ABS community - thus it is more about writing and not about unique research and programming, this has been done already at this point. this paper will help me very much in defining a basic structure of the thesis defining structure of thesis

April - August writing thesis publishing of papers

September holiday and moving to austria submitting thesis

TODO: update and adopt to 2nd year Papers route: end of march 2018: PFE paper, dependent types in ABS: march 2019 for ICFP 2019, towards pure functional abs paper as concept paper to the ABS Community until april 2019 (before starting thesis writing)

In this chapter we discuss in more detail how we plan to approach the aim and objectives stated in Chapter 4. Further we give a short overview of planned papers and present a Gantt-Chart 6.2 reflecting the most important activities and relevant milestones.

### 6.1 Approaching the Objectives

#### 6.1.1 Tools and foundations

In the first year a prototype of the library should be implemented with a few examples to early gain a good understanding of the topic and to be able to judge whether it is a dead-end or not. This has already successfully happened: the library prototype exists with a number of non-trivial examples including a full

implementation of the Sugarscape model. The library is termed FrABS<sup>1</sup> and is described in Appendix ??.

To be able to compare our approach to the existing state-of-the-art in the field of ABS we will use the existing library Repast Java. This will allow us to compare the dominant object-oriented paradigm in the field to our approach, discuss similarities and differences and identify draw benefits and drawbacks.

Clarification on the fundamental challenges in implementing ABS from a programming-paradigm agnostic perspective must be done. This was already conducted in the first paper on Update-Strategies in ABS, which is now accepted at SSC2017 and can be found in Appendix ??

### 6.1.2 Pure functional and object-oriented paradigms

The next objective is then to investigate the fundamental differences between the pure functional and object-oriented paradigms in implementing ABS with their respective incarnations Haskell and Java. This research will be conducted in the form of a report because it imposes no limits on content-size, is easier to be incorporated in the thesis than a paper and if required a paper can be condensed out of it. This work should pick up the work of the Update-Strategies paper and broaden and deepen its approach: show in more depth and in more detail which problems need to be solved when implementing an ABS and how both paradigms can be used in their way to solve them and identify potential benefits and drawbacks. There exists already code in Haskell and Java without any additional libraries (except JDK and Haskell's standard library called Prelude) produced for the Update-Strategies paper which can be used for this work. In the next step we need to go up the abstraction ladder and investigate how FrABS and Repast Java approach these problems and compare them from a programming paradigm perspective and identify potential benefits and drawbacks. As examples the SIR compartment model in epidemiology should be implemented both as a System-Dynamics and ABS 2D-spatial/network model. Also a full implementation of Sugarscape should be attempted in Repast Java<sup>2</sup>. The questions we want to answer in this objective are

- What are the approaches of pure functional and object-oriented programming to ABS?
- What are the benefits/drawbacks of Haskell and what are the benefits/drawbacks of Java in implementing ABS?
- Are the benefits/drawbacks orthogonal to each other e.g. are the weaknesses of one language the other languages strength?

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<sup>1</sup>Note that - despite it took quite some effort - this library in itself is no the contribution of this Ph.D. but just a means to an end which allows to research and investigate the objectives and research questions and substantiate the hypotheses.

<sup>2</sup>There exists already an implementation of Chapter II in the Repast Java Demo library upon which we can build.

- Are there things which are unique when doing Haskell in ABS and cannot be done in a Java approach and vice versa?

At least half of the second year will be allocated to this very important research as it lays the very foundations. We conjecture that the conclusion of this research will be that both approaches - paradigms and libraries - though solving specific problems different, are basically equally powerful in implementing the given examples and ABS in general with no fundamental impossibilities on either side. The main notable (but not fundamental) differences will be performance and memory-consumption, lines-of-code, expressiveness, usability, learning curve and they way to think about ABS. The question is then: why go through all the pain? Is there a difference? Can't we build somehow on the promised benefits of pure functional programming as in Haskell <sup>3</sup>?

### 6.1.3 Robustness and correctness

The answer to the previous question is attempted in a second study, which will look into how pure functional programming can increase robustness, testability, verification and correctness of Agent-Based Simulations. Again the approach will be in writing a report so not to restrict the size of the content, make it easier to incorporate it in the final thesis and condense a paper out of it if required. Again Repast Java and FrABS Haskell will be used as tools to investigate the research question by investigating the examples implemented in the previous report. The following investigations should be made:

- Compare the potential for bugs at runtime e.g. which are not possible to detect at compile time.
- Reproducibility robustness: can unpredictable side-effects affect the systems behaviour? Can such side-effects be guaranteed to not show up?
- Testing and testability of an implementation: how well can we test it using automated tests e.g. unit-tests, property-tests?
- Verification of an implementation: can we verify the correctness of a model or at least of parts of the specification?
- Can we establish a measure of correctness?

The second half of the 2nd year is allocated to this work.

We conjecture that this research will come to the conclusion that pure functional programming dramatically increases the robustness and correctness of an ABS and that it allows for easier and clearer approach to verification using specification testing in QuickCheck and automated testing using Unit- and Property-Testing.

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<sup>3</sup>Explicit about side-effects, strong static type-system, algebraic reasoning, declarative style, lambda calculus

### 6.1.4 Reasoning about dynamics

This objective investigates how far we can get using the pure functional paradigms' ability to reason about a program when applying it to reason about the dynamics of an ABS. As use-cases the idea is to look into reasoning about the equivalence of SD- and ABS-implementation of the SIR compartment model in epidemiology and about the equilibrium dynamics of the bilateral decentralized bartering in Sugarscape.

Both the System-Dynamics and Agent-Based implementation of the SIR compartment model in epidemiology lead to the same dynamics or put different: the Agent-Based implementation shows the same dynamics of the SD implementation when using replications. This is shown by plotting the dynamics as graphs.

In the Sugarscape model where agents engage in bilateral decentralized bartering equilibrium is only reached when neo-classical agents are used which don't die of natural age. The equilibrium is not reached when more realistic assumptions are made. This is shown by plotting the prices over time.

In this part of the Ph.D. we want to answer the following questions:

- What and to which extent can we reason about an Agent-Based Simulation in pure functional programming in general and using FrABS in particular?
- Can we show that the SD and ABS implementations are equivalent through reasoning about the code?
- Can we show that the equilibrium in the decentralized bilateral bartering of Sugarscape is reached / not reached when using neo-classical agents / realistic agents through reasoning about the code?

We are very well aware that this topic alone could justify a Ph.D. on its own and it is unsure if we would could make it this far (if the previous research takes longer than anticipated). Still we want to explicitly have clearly stated these objectives and outlined how to approach them - the worst which can happen is that they merely serve as a very in-depth outlook on future research. Thus the outcome of this research is highly uncertain but the conjecture is that we come to the following conclusion: it highly depends on the complexity and semantics of the model. In the case of the SIR compartment model we expect a success. In the case of the bilateral decentralized bartering in Sugarscape we probably will gain some insights but that at some point due to the interlocking of so many mechanisms it would get too complicated and a full and formal treatment is out of the scope of this Ph.D. We allocate the first half of the 3rd year to this work.

## 6.2 Planned Papers

For the remainder of the PhD we planned for two more papers. The first one will be focused on the pure functional approach to ABS, and targeted as a conference paper. Because we are doing interdisciplinary research which is a cross-over

between the fields of ABMS and functional programming in the theoretical computer sciences, we plan to write two papers on this same topic but for different audiences: one for the ABMS community and one for the field of functional programming. This would allow us to present our new concepts to two different groups and explain the same thing from two different perspectives. Also it would introduce the two groups to the ideas of the other group and may result in a cross-fertilization. The second paper we target as a journal paper and will focus on testing, verification and correctness in the functional approach to ABS. This paper will be written for the ABMS community and released in an ABMS journal.



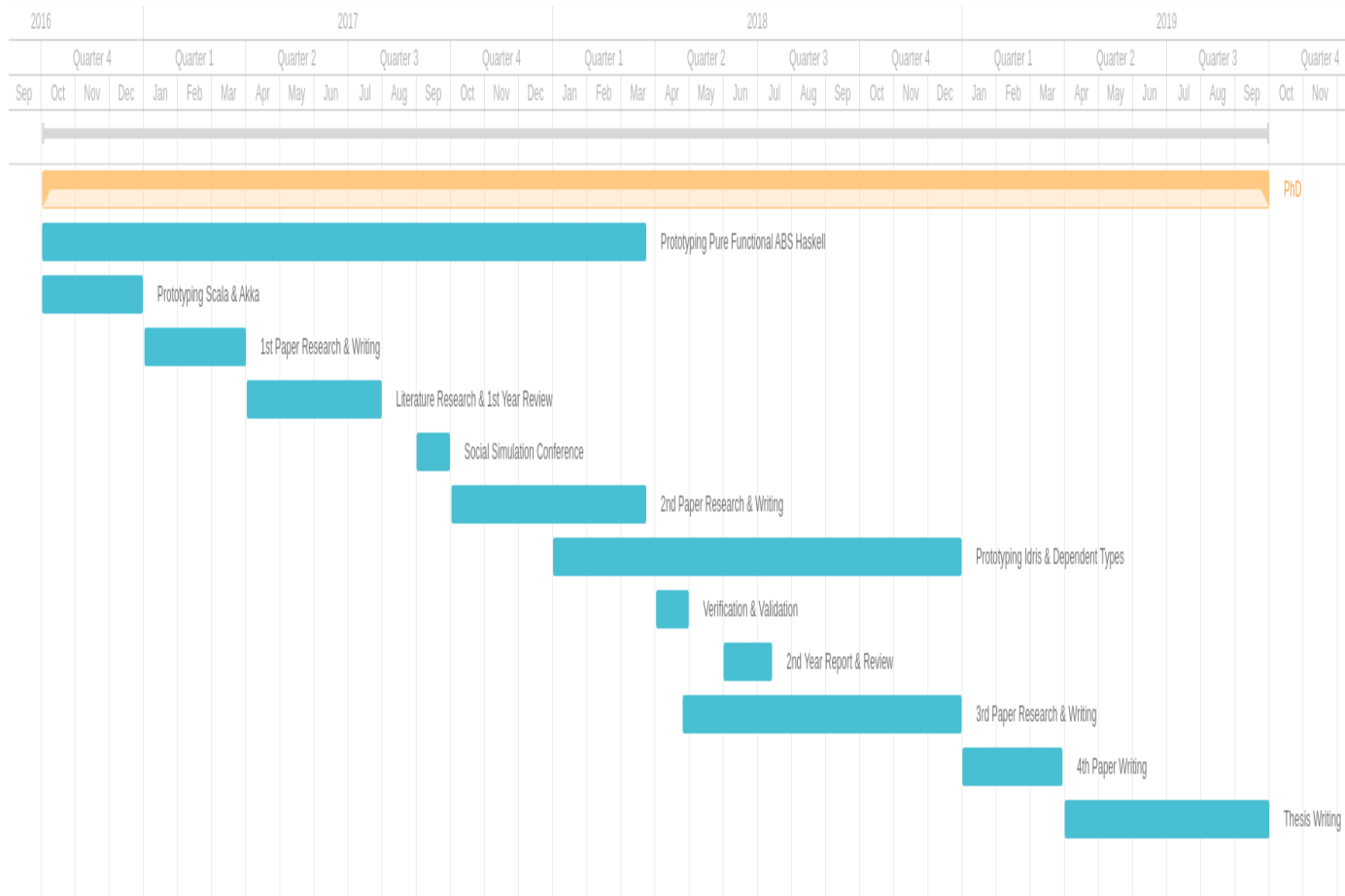


Figure 6.1: Gantt Chart of the PhD

## Chapter 7

# Conclusions

### 7.1 Being Realistic

It is of most importance to stress that we don't condemn the current state-of-the-art approach of object-oriented specification and implementation to ABS. The strength of object-oriented programming is surely that it can be seen as *programming as modelling* and thus will be always an attractive approach to ABS. Also we are realists and know that there are more points to consider when selecting a set of methods for developing software for an ABS than robustness, verification and validation. Almost always the popularity of an existing language and which languages the implementer knows is the driving force behind which methods and languages to choose. This means that ABS will continue to be implemented in object-oriented programming languages and many perfectly well functioning models will be created by it in the future. Although they all suffer from the same issues mentioned in the introduction this doesn't matter as they are not of central importance to most of them. Nonetheless we think our work is still essential and necessary as it may start a slow paradigm-shift and opens up the minds of the ABS community to a more functional and formal way of approaching and implementing agent-based models and simulations and recognizing the benefits one gets automatically from it by doing so.

### 7.2 What we are not doing

Because of this highly interdisciplinary topic we explicitly mention what we do not want to undertake in this PhD. First we don't want to develop another language for formal agent-specification which needs to be compiled or used in some fancy tool - we want to put it directly into Haskell, building on the existing facilities. Second, we are not developing a new economic theory about decentralized bilateral bartering, we take the existing theory and existing agent-based models and apply our methods to them. Third, we don't want to use fancy statistics and number juggling for comparing validating and verifying models: we want

structural comparison (category-theory). Fourth, we do NOT want to do a direct comparison of object-orientation vs. functional in ABS, as we would get lost in an infinite amount of low-level technical details. We look at the benefits / drawbacks more on a conceptual level, applied to ABS.

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# Appendices

## Appendix A

# Pure Functional Epidemics

- Submitted to Haskell Symposium 2018 on 30th March  
REJECTED on 18th May
- Submitted to IFL 2018 on 25th May  
NOTIFICATION PENDING until 20th July

# Pure Functional Epidemics

## An Agent-Based Approach

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### ABSTRACT

Agent-Based Simulation (ABS) is a methodology in which a system is simulated in a bottom-up approach by modelling the micro interactions of its constituting parts, called agents, out of which the global system behaviour emerges.

So far mainly object-oriented techniques and languages have been used in ABS. Using the SIR model of epidemiology, which simulates the spreading of an infectious disease through a population, we show how to use pure Functional Reactive Programming to implement ABS. With our approach we can guarantee the reproducibility of the simulation at compile time and rule out specific classes of run-time bugs, something that is not possible with traditional object-oriented languages. Also, we found that the representation in a purely functional format is conceptually quite elegant and opens the way to formally reason about ABS.

### KEYWORDS

Functional Reactive Programming, Monadic Stream Functions, Agent-Based Simulation

#### ACM Reference Format:

Jonathan Thaler, Thorsten Altenkirch, and Peer-Olaf Siebers. 2019. Pure Functional Epidemics: An Agent-Based Approach. In *Proceedings of International Symposium on Implementation and Application of Functional Languages (IFL '18)*. ACM, New York, NY, USA, 12 pages. <https://doi.org/10.1145/nnnnnnnn.nnnnnnnn>

## 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 [9] 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* [22] which still holds up today.

In this paper we challenge this metaphor and explore ways of approaching ABS in a pure (lack of implicit side-effects) functional way using Haskell. By doing this we expect to leverage the benefits of pure functional programming [12]: higher expressivity through

declarative code, being polymorph and explicit about side-effects through monads, more robust and less susceptible to bugs due to explicit data flow and lack of implicit side-effects.

As use case we introduce the SIR model of epidemiology with which one can simulate epidemics, that is the spreading of an infectious disease through a population, in a realistic way.

Over the course of four steps, we derive all necessary concepts required for a full agent-based implementation. We start from a very simple solution running in the Random Monad which has all general concepts already there and then refine it in various ways, making the transition to Functional Reactive Programming (FRP) [36] and to Monadic Stream Functions (MSF) [26].

The aim of this paper is to show how ABS can be implemented in *pure* Haskell and what the benefits and drawbacks are. By doing this we give the reader a good understanding of what ABS is, what the challenges are when implementing it and how we solve these in our approach.

The contributions of this paper are:

- We present an approach to agent-based simulation using *declarative* analysis with FRP in which we systematically introduce the concepts of ABS to *pure* functional programming in a step-by-step approach. Also this work presents a new field of application to FRP as to the best of our knowledge the application of FRP to ABS (on a technical level) has not been addressed before. 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. This only becomes possible in pure functional programming where we can control the side-effects and can program side-effect polymorph, 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

IFL '18, August 2019, Lowell, MA, USA

2019. ACM ISBN 978-x-xxxx-xxxx-x/YY/MM...\$15.00  
<https://doi.org/10.1145/nnnnnnnn.nnnnnnnn>



e.g. related to dynamic typing, and the lack of implicit data-dependencies which are common in traditional imperative object-oriented approaches.

In Section 2 we define agent-based simulation, introduce functional reactive programming, arrowized programming and monadic stream functions, because our approach builds heavily on these concepts. In Section 3 we introduce the SIR model of epidemiology as an example model to explain the concepts of ABS. The heart of the paper is Section 4 in which we derive the concepts of a pure functional approach to ABS in four steps, using the SIR model. Section 5 discusses related work. Finally, we draw conclusions and discuss issues in Section 6 and point to further research in Section 7.

## 2 BACKGROUND

### 2.1 Agent-Based Simulation

Agent-Based Simulation is 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 which can be understood as 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.

We informally assume the following about our agents [18, 30, 37]:

- 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 [8] 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.
- States - agents encapsulate some state which can be accessed and changed during the simulation.
- Feedback-Loops - because agents act continuously and their actions influence each other and themselves in subsequent time-steps, feedback-loops are the norm in ABS.
- Heterogeneity - although agents can have same properties like height, sex,... the actual values can vary arbitrarily between agents.
- Interactions - agents can be modelled after interactions with an environment or other agents.

- Spatiality & Networks - agents can be situated within e.g. a spatial (discrete 2D, continuous 3D,...) or complex network environment.

### 2.2 Functional Reactive Programming

Functional Reactive Programming 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 our approach we use *Arrowized FRP* [13, 14] as implemented in the library Yampa [4, 11, 21].

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  $\Delta t$  which are positive time-steps with which the system is sampled.

$$\begin{aligned} \text{Signal } \alpha &\approx \text{Time} \rightarrow \alpha \\ \text{SF } \alpha \beta &\approx \text{Signal } \alpha \rightarrow \text{Signal } \beta \end{aligned}$$

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. We shortly discuss the relevant combinators and concepts we use throughout the paper. For a more in-depth discussion we refer to [4, 11, 21].

*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, the combinator *switch*  $:: \text{SF } a (b, \text{Event } c) \rightarrow (c \rightarrow \text{SF } a \ b) \rightarrow \text{SF } a \ b$  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.

*Randomness.* In ABS one often needs to generate stochastic events which occur based on e.g. an exponential distribution. Yampa provides the combinator *occasionally*  $:: \text{RandomGen } g \Rightarrow g \rightarrow \text{Time} \rightarrow b \rightarrow \text{SF } a (\text{Event } b)$  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*  $:: (\text{RandomGen } g, \text{Random } b) \Rightarrow g \rightarrow \text{SF } a \ b$  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*  $:: \text{SF } a \ b \rightarrow (a, [(DTime, \text{Maybe } a)]) \rightarrow [b]$  which allows to run an SF for a given number of steps where in each step one provides the  $\Delta t$  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 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 [13, 14].

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 programming 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 [23] 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 [27].

```
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 Paterson's do-notation [23] 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.

### 2.4 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 [25, 26]:

```
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 Paterson's 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 => (a -> m b) -> MSF m a b* and *arrM\_* :: *Monad m => m b -> MSF m a b*.

## 3 THE SIR MODEL

To explain the concepts of ABS and of our pure functional approach to it, we introduce the SIR model as a motivating example and



Figure 1: States and transitions in the SIR compartment model.

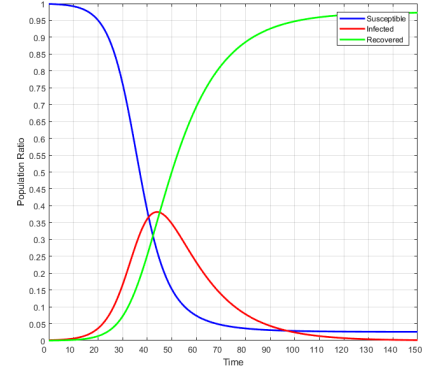


Figure 2: Dynamics of the SIR compartment model using the System Dynamics approach. Population Size  $N = 1,000$ , contact rate  $\beta = \frac{1}{5}$ , infection probability  $\gamma = 0.05$ , illness duration  $\delta = 15$  with initially 1 infected agent. Simulation run for 150 time-steps.

use-case for our implementation. It is a very well studied and understood compartment model from epidemiology [16] which allows to simulate the dynamics of an infectious disease like influenza, tuberculosis, chicken pox, rubella and measles spreading through a population [7].

In this model, people in a population of size  $N$  can be in either one of 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  $\beta$  other people per time-unit and become infected with a given probability  $\gamma$  when interacting with an infected person. When infected, a person recovers *on average* after  $\delta$  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 1.

This model was also formalized using System Dynamics (SD) [28]. 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. We won't go into detail here and provide the dynamics of such a solution for reference purposes, shown in Figure 2.

### An Agent-Based approach

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 by interactions amongst the agents

and time-outs. The major advantage of ABS is that it allows to incorporate spatiality as shown in Section 4.4 and simulate heterogeneity of population e.g. different sex, age. This is not possible with other simulation methods e.g. SD or Discrete Event Simulation (DES).

According to the model, every agent makes *on average* contact with  $\beta$  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 proportional to the size of the population [2]. 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.

This results in the following agent behaviour:

- *Susceptible*: A susceptible agent makes contact *on average* with  $\beta$  other random agents. For every *infected* agent it gets into contact with, it becomes infected with a probability of  $\gamma$ . If an infection happens, it makes the transition to the *Infected* state.
- *Infected*: An infected agent recovers *on average* after  $\delta$  time units. This is implemented by drawing the duration from an exponential distribution [2] with  $\lambda = \frac{1}{\delta}$  and making the transition to the *Recovered* state after this duration.
- *Recovered*: These agents do nothing because this state is a consuming state from which there is no escape: recovered agents stay immune and can not get infected again in this model.

## 4 DERIVING A PURE FUNCTIONAL APPROACH

We presented a high-level agent-based approach to the SIR model in the previous section, which focused only on the states and the transitions, but we haven't talked about technical implementation.

In [33] two fundamental problems of implementing an agent-based simulation from a programming-language agnostic point of view is discussed. The first problem is how agents can be pro-active and the second how interactions and communication between agents can happen. For agents to be pro-active, they must be able to perceive the passing of time, which means there must be a concept of an agent-process which executes over time. Interactions between agents can be reduced to the problem of how an agent can expose information about its internal state which can be perceived by other agents. Further the authors have shown the influence of different deterministic and non-deterministic elements in agent-based simulation on the dynamics and how the influence of non-determinism can completely break them down or result in different dynamics despite same initial conditions. This means that we want to rule out any potential source of non-determinism.

In this section we will derive a pure functional approach for an agent-based simulation of the SIR model in which we will pose solutions to the previously mentioned problems. We will start out with a very naive approach and show its limitations which we overcome by adding FRP. Then in further steps we will add more

concepts and generalisations, ending up at the final approach which utilises Monadic Stream Functions, a generalisation of FRP.

Of paramount importance is to keep our implementations pure which rules out the use of the IO Monad and thus any potential source of non-determinism under all circumstances because we would lose all compile time guarantees about reproducibility. Still we will make use of the Random and State Monad which indeed allow side-effects but the crucial point here is that we restrict side-effects only to these types in a controlled way without allowing general unrestricted effects <sup>1</sup>.

### 4.1 Naive beginnings

We start by modelling the states of the agents. Infected agents are ill for some duration, meaning we need to keep track when an infected agent recovers. Also a simulation is stepped in discrete or continuous time-steps thus we introduce a notion of *time* and  $\Delta t$  by defining:

```
type Time = Double
type TimeDelta = Double
```

```
data SIRState = Susceptible | Infected TimeDelta | Recovered
```

Now we can represent every agent simply as its SIR state. We hold all our agents in a list:

```
type SIRAgent = SIRState
type Agents = [SIRAgent]
```

Next we need to think about how to actually step our simulation. For this we define a function which advances our simulation with a fixed  $\Delta t$  until a given time  $t$  where in each step the agents are processed and the output is fed back into the next step. This is the source of pro-activity as agents are executed in every time step and can thus initiate actions based on the passing of time. Note that we step the simulation with a hard-coded  $\Delta t = 1.0$  for reasons which become apparent when implementing the *susceptible* behaviour. As already mentioned, the agent-based implementation of the SIR model is inherently stochastic which means we need access to a random-number generator. We decided to use the Random Monad at this point as threading a generator through the simulation and the agents would be very cumbersome. Thus our simulation stepping runs in the Random Monad:

```
runSimulation :: RandomGen g => Time -> Agents -> Rand g [Agents]
runSimulation tEnd as = runSimulationAux 0 as []
  where
    runSimulationAux :: RandomGen g
      => Time -> Agents -> [Agents] -> Rand g [Agents]
    runSimulationAux t as acc
      | t >= tEnd = return (reverse (as : acc))
      | otherwise = do
        as' <- stepSimulation as
        runSimulationAux (t + 1.0) as' (as : acc)

stepSimulation :: RandomGen g => Agents -> Rand g Agents
stepSimulation as = mapM (runAgent as) as
```

Now we can implement the behaviour of an individual agent. First we need to distinguish between the agents SIR states:

```
processAgent :: RandomGen g => Agents -> SIRAgent -> Rand g SIRAgent
processAgent as Susceptible = susceptibleAgent as
processAgent _ (Infected dur) = return (infectedAgent dur)
processAgent _ Recovered = return Recovered
```

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

An agent 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.

From our implementation it becomes apparent that only the behaviour of a susceptible agent involves randomness and that a recovered agent is simply a sink - it does nothing and stays constant.

Lets look how we can implement the behaviour of a susceptible agent. It simply makes contact on average with a number of other agents and gets infected with a given probability if an agent it has contact with is infected. Here it becomes apparent that we implicitly assume that the simulation is stepped with a  $\Delta t = 1.0$ . If we would use a different  $\Delta t$  then we need to adjust the contact rate accordingly because it is defined *per time-unit*. This would amount to multiplying with the  $\Delta t$  which in combination with the discretisation using *floor* would lead to too few contacts being made, ultimately resulting in completely wrong dynamics.

When the agent gets infected, it calculates also its time of recovery by drawing a random number from the exponential distribution, meaning it is ill on average for *illnessDuration*.

```
susceptibleAgent :: RandomGen g => Agents -> Rand g SIRAgent
susceptibleAgent as = do
  -- draws from exponential distribution
  rc <- randomExpM (1 / contactRate)
  cs <- replicateM (floor rc) (makeContact as)
  if or cs
  then infect
  else return Susceptible
where
  makeContact :: RandomGen g => Agents -> Rand g Bool
  makeContact as = do
    randContact <- randomElem as
    case randContact of
      -- returns True with given probability
      (Infected _) -> randomBoolM infectivity
      _              -> return False

  infect :: RandomGen g => Rand g SIRAgent
  infect = randomExpM (1 / illnessDuration)
  >>= \rd -> return (Infected rd)
```

The infected agent is trivial. It simply recovers after the given illness duration which is implemented as follows:

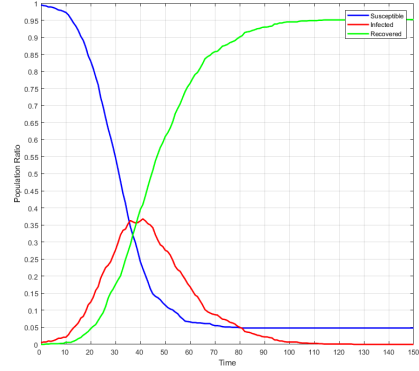
```
infectedAgent :: TimeDelta -> TimeDelta -> SIRAgent
infectedAgent dur
  | dur' <= 0 = Recovered
  | otherwise = Infected dur'
where
  dur' = dur - 1.0
```

Again note the hard-coded  $\Delta t = 1.0$ .

**4.1.1 Results.** When running our naive implementation with a population size of 1,000 we get the dynamics as seen in Figure 3. When comparing it to the dynamics of the reference in Figure 2, the agent-based dynamics are not as smooth which stems from the fact that the agent-based approach is inherently discrete and stochastic [17].

**4.1.2 Discussion.** Reflecting on our first naive approach we can conclude that it already introduced most of the fundamental concepts of ABS

- Time - the simulation occurs over virtual time which is modelled explicitly divided into *fixed*  $\Delta t$  where at each step all agents are executed.
- Agents - we implement each agent as an individual, with the behaviour depending on its state.



**Figure 3: Naive simulation of SIR using the agent-based approach. Population of 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 with fixed  $\Delta t = 1.0$ .**

- 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 Monad type and the usage of *randomBoolM* and *randomExpM*.
- 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 in the Random Monad and *not* in the IO Monad. This guarantees that no external, uncontrollable sources of non-determinism can interfere with the simulation.

Nonetheless our approach has also weaknesses and dangers:

- (1) We are using a hard-coded  $\Delta t = 1.0$  because of the way our susceptible behaviour is implemented. Also  $\Delta t$  is dealt with explicitly in the infected behaviour where it is hard-coded to  $\Delta t = 1.0$ . This is not very modular and elegant and a potential source of errors - can we do better and find a more elegant solution?
- (2) The way our agents are represented is not very modular. The state of the agent is explicitly encoded in an ADT and when processing the agent, the behavioural function always needs to distinguish between the states. Can we express it in a more modular way e.g. continuations?

We now move on to the next section in which we will address these points.

## 4.2 Adding Functional Reactive Programming

As shown in the first step, the need to handle  $\Delta t$  explicitly can be quite messy, is inelegant and a potential source of errors, also the explicit handling of the state of an agent and its behavioural function is not very modular. We can solve both these weaknesses



by switching to the Functional Reactive Programming paradigm, because it allows to express systems with discrete and continuous time-semantics.

In this step we are focusing on Arrowized FRP [13] using the library Yampa [11]. In it, time is handled implicitly, meaning it cannot be messed with, which is achieved by building the whole system on the concept of signal functions (SF). An SF can be understood as a process over time and is technically a continuation which allows to capture state using closures. Both these fundamental features allow us to tackle the weaknesses of our first step and push our approach further towards a truly elegant functional approach.

**4.2.1 Implementation.** We start by re-defining the SIR states, whereas now the illness duration is not needed any more. Also we re-define an agent to be an SF which receives the SIR states of all agents as input and outputs the SIR state of the agent:

```
data SIRState = Susceptible | Infected | Recovered
```

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

Now we can define the behaviour of an agent to be the following:

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

Depending on the initial state we return the corresponding behaviour. Most notably is the difference that we are now 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 which is in accordance with the implementation in the previous step where it acts as a sink which returns constantly the same state:

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

When an event occurs we can change the behaviour of an agent using the Yampa combinator *switch*, which is much more elegant and expressive than the initial approach as it makes the change of behaviour at the occurrence of an event explicit. 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. Instead of randomly drawing the number of contacts to make, we now follow a fundamentally different approach by using Yampas *occasionally* function. This requires us to carefully select the right  $\Delta t$  for sampling the system as will be shown in results.

```
susceptibleAgent :: RandomGen g => g -> SIRAgent
susceptibleAgent g =
  switch (susceptible g) (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
        a <- drawRandomElemSF g -< as
        case a of
          Infected -> do
            i <- randomBoolSF g infectivity -< ()
            if i
            then returnA -< (Infected, Event ())
            else returnA -< (Susceptible, NoEvent)
```

```
- -> returnA -< (Susceptible, NoEvent))
else returnA -< (Susceptible, NoEvent)
```

We deal with randomness differently now and implement 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 needs 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)
```

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 infected (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)
```

Running and stepping the simulation works now a bit differently, using 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, [4, 21] 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 because in Yampa switching occurs immediately at  $t = 0$ . If we don't delay the switching at  $t = 0$  until the next step, we would enter an infinite switching loop - *notYet* simply delays the first switching until the next time-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, ignored at t = 0
  (switchingEvt >>> notYet)
  -- recursively switch back into stepSimulation
  stepSimulation
  where
    switchingEvt :: SF ((), [SIRState]) (Event [SIRState])
    switchingEvt = arr (\ (_, newAs) -> Event newAs)
```



**Figure 4: FRP simulation of agent-based SIR showing the influence of different  $\Delta t$ . 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  $\Delta t$ .**

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. The `d` in `dpSwitch` stands for decoupled which guarantees that it delays the switching until the next time-step: the function into which we switch is only applied in the next step, which prevents an infinite loop if we switch into a recursive continuation.

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.

**4.2.2 Results.** The dynamics generated by this step can be seen in Figure 4.

In this step we followed the FRP approach which is fundamentally different from the previous step in Section 4.1 because in FRP we assume a continuous flow of time as opposed to discrete time-steps of  $\Delta t = 1.0$  previously. This means that we need to select a *correct*  $\Delta t$  otherwise we would end up with wrong dynamics. The selection of a correct  $\Delta t$  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  $\Delta t$



**Figure 5: 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  $\Delta t$  or super-sampling all 3 events can be captured.**

which matches the frequency of events generated by *contact rate*. If we choose a too large  $\Delta t$ , we lose events which will result in wrong dynamics as can be seen in Figure 4a. This issue is known as under-sampling and is described in Figure 5.

For tackling this issue we have two options. The first one is to use a smaller  $\Delta t$  as can be seen 4b, which results in the whole system being sampled more often, thus reducing performance. The other option is to implement super-sampling and apply it to *occasionally* which would allow us to run the whole simulation with  $\Delta t = 1.0$  and only sample the *occasionally* function with a much higher frequency.

An approach to super-sampling would be to introduce a new combinator to Yampa which allows us to super-sample other signal functions.

```
superSampling :: Int -> SF a b -> SF a [b]
```

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. We have investigated super-sampling more in-depth but have to omit this due to lack of space.

**4.2.3 Discussion.** By moving on to FRP using Yampa we made a huge improvement in clarity, expressivity and robustness of our implementation. State is now implicitly encoded, depending on which signal function is active. Also by using explicit time-semantics with *occasionally* we can achieve extremely fine grained stochastics. Compared to drawing a random number of events we create only a single event or none at all. This requires to sample the system with a much smaller  $\Delta t$  than in the previous step: we are treating it as a truly continuous agent-based system.

A very severe problem, very 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 solution would be to simply split the initial random-number generator in *sirAgent* three times (using one of the splitted generators for the next split) and pass three random-number generators to *susceptible*. Note that this is not an issue in Sections 4.1 and 4.3 as we are using the Random Monad, which never uses the same random-number generator twice thus resulting in guaranteed uncorrelated stochastics.

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. To conveniently introduce it we want to make use of monads which is not possible using Yampa. In the next step we make the transition to Monadic Stream Functions as introduced in Dunai [26] which allows FRP within a monadic context.

### 4.3 Generalising to Monadic Stream Functions

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, which we will need in the next step when adding an environment.

**4.3.1 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, except from a few type-declarations, because BearRiver re-implements all necessary functions we are using from Yampa. We simply re-define our agent signal function, introducing the monad stack our SIR implementation runs in:

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

**4.3.2 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 get rid of the RandomGen arguments to our functions and run the whole simulation within the Random Monad *again* just as we started but now with the full features functional reactive programming. 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)
```

**4.3.3 Discussion.** So far making the transition to MSFs does not seem as compelling as making the move from the Random



**Figure 6: Common neighbourhoods in discrete 2D environments of Agent-Based Simulation.**

Monad to FRP in the beginning. Running in the Random Monad within FRP is convenient but we could achieve the same by passing RandomGen around as we already demonstrated. Still it guarantees us that we won't have correlated stochastics as discussed in the previous section. In the next step we introduce the concept of a read/write environment which we realise using a StateT monad. This will show the real benefit of the transition to MSFs.

### 4.4 Adding an environment

In this step we will add an environment in which the agents exist and through which they interact with each other. This is a fundamentally different approach to agent interaction but is as valid as the approach in the previous steps.

In ABS agents are often situated within a discrete 2D environment [9] which is simply a finite  $N \times M$  grid with either a Moore or von Neumann neighbourhood (Figure 6). 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 environment. Also instead of feeding back the states of all agents as inputs, agents now communicate through the environment by revealing their current state to their neighbours by placing it on their cell. Agents can read the states of all their neighbours which tells them if a neighbour is infected or not. For purposes of a more interesting approach, we restrict the neighbourhood to Moore (Figure 6b).

**4.4.1 Implementation.** We start by defining our discrete 2D environment for which we use an indexed two dimensional array. In each cell the agents will store their current state, thus we use the *SIRState* as type for our array data:

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

Next we redefine our monad stack and agent signal function. We use a StateT transformer on top of our Random Monad from the previous step with *SIREnv* as type for the state. Our agent signal function now has unit input and output type, which indicates that the actions of the agents are only visible through side-effects in the monad stack they are running in.

```
type SIRMonad g = StateT SIREnv (Rand g)
type SIRAgent g = SF (SIRMonad g) () ()
```

The implementation of a susceptible agent is now a bit different. The agent directly queries the environment for its neighbours and randomly selects one of them. The remaining behaviour is similar:

```

929 susceptibleAgent :: RandomGen g => Disc2dCoord -> SIRAgent g
930 susceptibleAgent coord
931   = switch susceptible (const (infectedAgent coord))
932   where
933     susceptible :: RandomGen g
934     => SF (SIRMonad g) () ((), Event ())
935     susceptible = proc _ -> do
936       makeContact <- occasionallyM (1 / contactRate) () <- ()
937       if not (isEvent makeContact)
938       then returnA <- ((), NoEvent)
939       else do
940         env <- arrM_ (lift get) <- ()
941         let ns = neighbours env coord agentGridSize moore
942         s <- drawRandomElemS <- ns
943         case s of
944           Infected -> do
945             infected <- arrM_
946               (lift $ lift $ randomBoolM infectivity) <- ()
947             if infected
948             then do
949               arrM (put . changeCell coord Infected) <- env
950               returnA <- ((), Event ())
951             else returnA <- ((), NoEvent)
952           _ -> returnA <- ((), NoEvent)
953
954 neighbours :: SIREnv -> Disc2dCoord -> Disc2dCoord
955           -> [Disc2dCoord] -> [SIRState]
956
957 moore :: [Disc2dCoord]
958 moore = [ topLeftDelta, topDelta, topRightDelta,
959           leftDelta, rightDelta,
960           bottomLeftDelta, bottomDelta, bottomRightDelta ]
961
962 topLeftDelta :: Disc2dCoord
963 topLeftDelta = (-1, -1)
964 topDelta :: Disc2dCoord
965 topDelta = (0, -1)
966 ...

```

Querying the neighbourhood is done using the *neighbours* function. It takes the environment, the coordinate for which to query the neighbours for, the dimensions of the 2D grid and the neighbourhood information and returns the data of all neighbours it could find. Note that on the edge of the environment, it could be the case that fewer neighbours than provided in the neighbourhood information will be found due to clipping.

The behaviour of an infected agent is similar to in the previous step, with the difference that upon recovery the infected agent updates its state in the environment from Infected to Recovered.

Running the simulation with MSFs works slightly different. The function *embed* we used before is not provided by BearRiver but by Dunai which has important implications. 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  $\Delta t$ . This is the reason why we need lifts e.g. in case of getting the environment. Thus *embed* returns a computation in the ReaderT Double Monad which we need to peel away using *runReaderT*. This then results in a StateT computation which we evaluate by using *evalStateT* and an initial environment as initial state. This then results in another monadic computation of the Random Monad type which we evaluate using *evalRand* which delivers the final result. Note that instead of returning agent states we simply return a list of environments, one for each step. The agent states can then be extracted from each environment.

```

982 runSimulation :: RandomGen g => g -> Time -> DTime
983           -> SIREnv -> [(Disc2dCoord, SIRState)] -> [SIREnv]
984 runSimulation g t dt env as = evalRand esRand g
985   where
986     steps = floor (t / dt)

```



**Figure 7: Simulating the agent-based SIR model on a 21x21 2D grid with Moore neighbourhood (Figure 6b), a single infected agent at the center and same SIR parameters as in Figure 2. Simulation run until  $t = 200$  with fixed  $\Delta t = 0.1$ . Last infected agent recovers shortly after  $t = 160$ . The susceptible agents are rendered as blue hollow circles for better contrast.**

```

dts      = replicate steps ()
-- initial SFs of all agents
sfs      = map (uncurry sirAgent) as
-- running the simulation
esReader = embed (stepSimulation sfs) dts
esState  = runReaderT esReader dt
esRand   = evalStateT esState env

```

Due to the different approach of returning the SIREnv in every step, we implemented our own MSF:

```

stepSimulation :: RandomGen g
=> [SIRAgent g] -> SF (SIRMonad g) () SIREnv
stepSimulation sfs = MSF (\_ -> do
  -- running all SFs with unit input
  res <- mapM (\unMSF -> ()) sfs
  -- extracting continuations, ignore output
  let sfs' = fmap snd res
  -- getting environment of current step
  env <- get
  -- recursive continuation
  let ct = stepSimulation sfs'
  return (env, ct))

```

**4.4.2 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 7.

Note that the dynamics of the spatial SIR simulation which are seen in Figure 7b look quite different from the reference dynamics of Figure 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.

**4.4.3 Discussion.** At first the environment approach might seem a bit overcomplicated and one might ask what we have gained by using an unrestricted neighbourhood where all agents can contact all others. The real advantage is that we can introduce arbitrary restrictions on the neighbourhood as shown with the Moore neighbourhood.

Of course 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 StateT monad and provide corresponding neighbourhood querying functions. The ability to place the heterogeneous agents in a generic environment is also the fundamental advantage of an agent-based over other simulation approaches and allows us to simulate much more realistic scenarios.

## 4.5 Additional Steps

ABS involves a few more advanced concepts which we don't fully explore in this paper due to lack of space. Instead we give a short overview and discuss them without presenting code or going into technical details.

**4.5.1 Agent-Transactions.** Agent-transactions are necessary when an arbitrary number of interactions between two agents need to happen instantaneously without time-lag. The use-case for this are price negotiations between multiple agents where each pair of agents needs to come to an agreement in the same time-step [9]. In object-oriented programming, the concept of synchronous communication between agents is implemented directly with method calls.

We have implemented synchronous interactions, which we termed agent-transactions in an additional step. We solved it pure functionally by running the signal functions of the transacting agent pair as often as their protocol requires but with  $\Delta t = 0$ , which indicates the instantaneous character of agent-transactions.

**4.5.2 Event Scheduling.** Our approach is inherently time-driven where the system is sampled with fixed  $\Delta t$ . The other fundamental way to implement an ABS in general, is to follow an event-driven approach [20] which is based on the theory of Discrete Event Simulation [38]. In such an approach the system is not sampled in fixed  $\Delta t$  but advanced as events occur where the system stays constant in between. Depending on the model, in an event-driven approach it may be more natural to express the requirements of the model.

In an additional step we have implemented a rudimentary event-driven approach which allows the scheduling of events but had to omit it due to lack of space. Using the flexibility of MSFs we added a State transformer to the monad stack which allows enqueueing of events into a priority queue. The simulation is advanced by processing the next event at the top of the queue which means running the MSF of the agent which receives the event. The simulation terminates if there are either no more events in the queue or after a given number of events, or if the simulation time has advanced to some limit. Having made the transition to MSFs, implementing this feature was quite straight forward which shows the power and strength of the generalised approach to FRP using MSFs.

**4.5.3 Dynamic Agent creation.** In the SIR model, the agent population stays constant - agents don't die and no agents are created during simulation - but some simulations [9] require dynamic agent creation and destruction. We can easily add and remove agents signal functions in the recursive switch after each time-step. The only problem is that creating new agents requires unique agent ids but with the transition to MSFs we can add a monadic context which allows agents to draw the next unique agent id when they create a new agent.

## 5 RELATED WORK

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 and look into how agents can be specified using the belief-desire-intention paradigm [6, 15, 32].

A library for DES and SD in Haskell called *Aivika 3* is described in the technical report [31]. It is not pure, as it uses the IO Monad under the hood and comes only with very basic features for event-driven ABS, which allows to specify simple state-based agents with timed transitions.

Using functional programming for DES was discussed in [15] where the authors explicitly mention the paradigm of FRP to be very suitable to DES.

A domain-specific language for developing functional reactive agent-based simulations was presented in [35]. 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 Yampa 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 [5] 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 [10]. 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 4.4. 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.

## 6 CONCLUSIONS

Our approach is radically 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  $\Delta t$  should be. Third it requires one to think about agent interactions in a new way instead of being just method-calls.

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 and State 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  $\Delta t$  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 [27]. Also by using FRP we gain all the benefits from it and can use research on testing, debugging and exploring FRP systems [24, 27].

## Issues

Currently, the performance of the system is not comparable to imperative implementations but our research was not focusing on this aspect. We leave the investigation and optimization of the performance aspect of our approach for further research.

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 [29] 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 an agent can be hidden behind a polymorphic interface which is much more abstract than in our approach. Also the identity of an agent is much clearer in object-oriented programming due to the concept of object-identity and the encapsulation of data and methods.

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 straight-forward 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 have added further mechanisms of agent interaction which we had to omit due to lack of space.

## 7 FURTHER RESEARCH

We see this paper 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 [1, 19, 34].

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 [3] 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 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:

- Accessing the environment in section 4.4 involves indexed array access which is always potentially dangerous as the indices have to be checked at run-time. Using dependent types it should be possible to encode the environment dimensions into the types. In combination with suitable data types for coordinates one should be able to ensure already at compile time that access happens only within the bounds of the environment.
- In the SIR implementation one could make wrong state-transitions e.g. 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 many agent-based models define their agents in terms of state-machines.
- An infected agent recovers after a given time - the transition of infected to recovered is a timed transition. Nothing prevents us from *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.
- 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 our implementation, we terminate the SIR model always after a fixed number of time-steps. We can informally reason that restricting the simulation to a fixed number of time-steps is not necessary because the SIR model *has to* reach a steady state after a finite number of steps. This means that at that point the dynamics won't change any more, thus one can safely terminate the simulation. Informally speaking,

the reason for that is that eventually the system will run out of infected agents, which are the drivers of the dynamic. We know that all infected agents will recover after a finite number of time-steps *and* that there is only a finite source for infected agents which is monotonously decreasing. Using dependent types it might be possible to encode this in the types, resulting 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.

## ACKNOWLEDGMENTS

The authors would like to thank I. Perez, H. Nilsson, J. Greensmith, M. Baerenz, H. Vollbrecht, S. Venkatesan and J. Hey for constructive feedback, comments and valuable discussions.

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Received May 2018

# Appendix B

## Questions & Answers

In this chapter I give answers to anticipated questions and objections about my research direction and vision of doing pure functional ABS <sup>1</sup>.

**So you had this hypothesis, that pure functional programming and dependent types lead to simulation software which is more likely correct and is easier to verify and validate, right from the beginning?**

Not at all. I even had no deep knowledge of functional programming at the start of my PhD, I've just worked through the 1st edition of Grahams book "Programming in Haskell" and that's it. I had no clear understanding of purity, side-effects and Monads and I didn't know a bit about functional reactive programming. I knew that something like Dependent Types exist because Thorsten (2nd Supervisor) has sent me an email before the start of my PhD in which he pointed at Agda, so I started reading a bit about intuitionistic / constructivistic math, tried out a little bit of Agda but quickly gave up because it was way too far away (without really having mastered pure functional programming in Haskell, I believe it is nearly impossible / too difficult / makes no sense going into dependent types). So in the beginning there was pure *curiosity* about functional programming in combination with ABS because I knew nothing of FP at all and wanted to understand it (after getting bored by OO) and applying FP to ABS seemed so crazy (because everyone claims OO to be 'natural' for it) that it must be an extremely interesting challenge. I guess this is very often the case with research: there is 'just' curiosity in the beginning and then during the research process a hypothesis falls into place.

**What is it with these weird dependent types? Why should we use them? Why are you so obsessed with strongly statically typed languages? How can we benefit from types? Aren't they just in our way?**

---

<sup>1</sup>They are not always posed in a dead-serious way but as it is a quite controversial topic - ABS should be done object-orientated after all huh? - I think it is appropriate. Also some objections were raised in exactly this way.

I understand that in the beginning when one learns a strong statically typed language, types seem often to get in ones way of doing things - it happened to me when I was learning Haskell and it is now the same issue as I am getting into Idris: types seem to restrict ones freedom instead of 'just letting one do' things one know are correct or work anyway.

The restriction 'complaint' is correct, types *do* restrict one and this is their main purpose because when these restrictions are used in a clever and appropriate way, they can be seen as an additional ingredient to programming which guide one in the program construction process by directing one and telling what is allowed and what is not. Well constructed programs and good libraries in strongly statically typed languages use types in exactly that way: to guide the programmer towards a better solution - by just looking at the types of a function one can derive very much about its intended use. It is almost always the case that when you are trying to work around the types, you are making a mistake.

In general, Types guide us in program construction by restricting the operations we can perform on the data. This means that by choosing types this reveals already a lot of our program and data and prevents us from making mistakes e.g. interpreting some binary data as text instead of a number. In strongly statically typed languages the types can do this already at compile time which allows to rule out certain bugs already at compile time. In general, we can say that for all bugs which can be ruled out at compile time, we don't need to write property- or unit-tests for them, because those bugs cannot - per definition - occur at run-time, so it won't make sense to test their absence at run-time. Also, as Dijkstra famously put it: "Testing shows the presence, not the absence of bugs" - thus by induction we can claim that compile time guarantees save us from a potentially infinite amount of testing.

Dependent types allow to push these guarantees to a new extreme where we can express nearly arbitrary complex guarantees at compile time because we can *compute types at compile time*. The main requirement here is, that the computation is total. So dependent types go as far as seen as equivalent to mathematical proofs, which in the end allows to guarantee so much properties at compile time so as to make it unnecessary to run the program because the compilation already shows its correctness.

So short answer: types allow us to guarantee things at compile time which reduces the amount of testing considerably.

**You said by implementing a few different models with your functional approach showed you that it is very possible. You didn't say how hard or weird it was to achieve this - have you compared it to the object-oriented approach?** No I haven't compared it and I won't because there are hardly objective measures of how hard something is to implement in a paradigm. One could use the length of the program (Lines Of Code LoC) as a measure but then clearly the functional approach would win as functional code tends to be much shorter than object-oriented one with up to an order of magnitude.

Also I can pose a fundamentally challenging view: why should the object-oriented be regarded as the easier/better one? Just because oo is the established method doesn't make it the easier one, it hasn't really proved itself on an objective level that it is easier / less weird. Also I claim that some object-oriented constructs are VERY weird and VERY hard to get right (patterns, data-dependencies, inheritance, is-a vs. has-a, composition) without lots of experience.