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A tale of lock-free Agents: Towards Software Transactional Memory in parallel Agent-Based Simulation

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Abstract

With the decline of Moore's law and the ever increasing availability of cheap massively parallel hardware, it becomes more and more important to embrace parallel programming methods to implement Agent-Based Simulations (ABS). This has been acknowledge in the field a while ago and numerous research on distributed parallel ABS exists, focusing primarily on Parallel Discrete Event Simulation as the underlying mechanism. However, these concepts and tools are inherently difficult to master and apply and often overkill in case implementers simply want to parallelise their own, custom agent-based model implementation. However, with the established programming languages in the field, Python, Java and C++, it is not easy to address the complexities of parallel programming due to unrestricted side effects and the intricacies of low-level locking semantics. Therefore, in this paper we propose the use of a lock-free approach to parallel ABS using Software Transactional Memory (STM) in conjunction with the pure functional programming language Haskell, which in combination, removes some of the problems and complexities of parallel implementations in imperative approaches.

We present two case studies where we compare the performance of lock-based and lock-free STM implementations in two different well known Agent-Based Models, where we investigate both the scaling performance under increasing number of CPUs and the scaling performance under increasing number of agents. We show that the lock-free STM implementations consistently outperform the lock-based ones and scale much better to increasing number of CPUs both on local machines and on Amazon Cloud Services. Further, by utilizing the pure functional language Haskell we gain the benefits of immutable data and lack of unrestricted side effects guaranteed at compile-time, making validation easier and leading to increased confidence in the correctness of an implementation, something of fundamental importance and benefit in parallel programming in general and scientific computing like ABS in particular.

Keywords: Agent-Based Simulation; Software Transactional Memory; Parallel Programming; Haskell

1 Introduction

The future of scientific computing in general and Agent-Based Simulation (ABS) in particular is parallelism: Moore's law is declining as we are reaching the physical limits of CPU clocks. The only option is going massively parallel due to availability of cheap massive parallel local hardware with many cores, or cloud services like Amazon EC. This trend has been already recognised in the field of ABS as a research challenge for *Large-scale ABMS* [1] was called out and as a substantial body of research for parallel ABS shows [2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13].

In this body of work it has been established that parallelisation of autonomous agents, situated in some spacial, metric environment can be particularly challenging. The reason for this is that the environment constitutes a key medium for the agents interactions, represented as a *passive* data structure, recording attributes of the environment and the agents [4]. Thus the problem of parallelising ABS boils down to the problem of how to synchronise access to shared state without violating the causality principle and resource constraints [3, 2]. Various researchers have developed different techniques where most of them are based on the concept of Parallel Discrete-Event Simulation (PDES). The idea behind PDES is to partition the shared space into logical processes which run at their own speed, processing events coming from themselves and other logical processes. To deal with inconsistencies there exists a conservative approach which does not allow to process events with a lower timestamp than the current time of the logical process; and an optimistic approach which deals with inconsistencies through rolling back changes to state.

Adopting PDES to ABS is challenging as agents are autonomous and thus the topology can change in every step, making it hard to predict the topology of logical processes in advance [4] and thus posing a difficult problem for parallelisation in general [13]. The work [2, 5] discusses this challenge by giving a detailed and in-depth discussion of the internals and implementation of their powerful and highly complex PDES-MAS system. The rather conceptual work [3] proposes a general, distributed simulation framework for multiagent systems and addresses a number of key problems: decomposition of the environment, load balancing, modelling, communication and shared state variables, which the authors mention as the central problem of parallelisation.

In addition, various distributed simulation environments for ABS have been developed and their internals published in research papers: the SPADES system [6] manages agents through UNIX pipes using a parallel sense-think-act cycle employing a conservative PDES approach; Mace3J [7] a Java based system running on single- or multicore workstations implements a message passing approach to parallelism; James II [8] is also a Java based system and focuses on PDEVS simulation with a plugin architecture to facilitate reuse of models; the well known RePast-HPC [9, 10] framework is using a PDES engine under the hood.

The baseline of this body of research is that parallelisation is possible and we know how to do it. However, the complexity of these parallel and distributed simulation concepts and toolkits is high and the model development effort is hard [12]. Further, this sophisticated and powerful machinery is not always required as ABS does not always need to be run in a distributed way but the implementers 'simply' want to parallelise their models locally. Although these existing distributed ABS frameworks could be used for this, they are overkill and more straightforward concepts for parallelising ABS would be appropriate. However, for this case there does not exist much research, and implementers either resort to the distributed ABS frameworks, implement their own low-level concurrency plumbing which can be considerably complex - or simply refrain from using parallelism due to the high complexity involved and accept a longer execution time. What makes it worse is that parallelism always comes with danger of additional, very subtle bugs, which might lie dormant, potentially invalidating significant scientific results of the model. Therefore something simpler is needed for local parallelism. Unfortunately, the established imperative languages in the ABS field, Python, Java, C++, don't make adding parallelism easy, due to their inherent use of unrestricted side effects. Further, they mostly follow a lock-based approach to concurrency which is error prone and does not compose.

This paper proposes Software Transactional Memory (STM) in conjunction with functional programming in Haskell [14] as a new underlying concept for local parallelisation of ABS. We hypothesise that by using STM in Haskell, implementing local parallel ABS is considerably easier than with lock-based approaches, less error prone and easier to validate. Although STM exists in other languages as well by now, Haskell was one of the first to natively build it into its core. Further, it has the unique benefit that it can guarantee the lack of persistent side effects at compile time, allowing unproblematic retries of transactions, something of fundamental importance in STM. This makes the use of STM in Haskell very compelling. Our hypothesis is supported by [15], which gives a good indication how difficult and complex constructing a correct concurrent program is and shows how much easier, concise and less error-prone an STM implementation is over traditional locking with mutexes and semaphores. Further, it shows that STM consistently outperforms the lock-based implementation.

To the best of our knowledge we are the first to *systematically* discuss the use of STM in the context of ABS. However, the idea of applying transactional memory to simulation in general is not new and was already explored in the work [11], where the authors looked into how to apply Intel's *hardware* transactional memory to simulations in the context of a Time Warp PDES simulation. The results showed that their approach generally outperformed traditional locking mechanisms.

The master thesis [16] investigates Haskells' parallel and concurrency features to implement (amongst others) *HLogo*, a Haskell clone of the NetLogo [17] simulation package, focusing on using STM for a limited form of agent interactions. *HLogo* is basically a re-implementation of NetLogos API in Haskell where agents run within an unrestricted side effect context (known as `IO`) and thus can also make use of STM functionality. The benchmarks show that this approach does indeed result in a speedup especially under larger agent populations. Despite the parallelism aspect our work share, our approach is rather different: we avoid unrestricted side effects through `IO` within the agents under all costs and explore the use of STM more on a conceptual level rather than implementing an ABS library.

The aim of this paper is to experimentally investigate the benefits of using STM over lock-based approaches for concurrent ABS models. Therefore, we follow [15] and compare the performance of lock-based and STM implementations and expect that the reduced complexity and increased performance will be directly applicable to ABS as well. We present two case studies in which we employ an agent-based spatial SIR [18, 19] and the well known SugarScape [20] model to test our hypothesis. The latter model can be seen as one of the most influential exploratory models in ABS which laid the foundations of object-oriented implementation of agent-based models. The former one is an easy-to-understand explanatory model which has the advantage that it has an analytical theory behind it which can be used for verification and validation.

The contribution of this paper is a systematic investigation of the usefulness of STM over lock-based approaches, therefore giving implementers a new method of locally parallelising their own implementations without the overhead of a distributed, parallel PDES system or the error-prone low-level locking semantics of a custom built parallel implementation. Therefore, our paper directly addresses the *Large-scale ABMS* challenge [1], which focuses on efficient modelling and simulating large-scale ABS. Further, using STM, which restricts side effects, and makes parallelism easier, can help in the validation challenge [1] *H5: Requirement that all models be completely validated.*

We start with Section 2 where we discuss the concepts of STM and side effects in Haskell. In Section 3 we show how to apply STM to ABS in general. Section 4 contains the first case study using a spatial SIR mode whereas Section 5 presents the second case study using the SugarScape model. We conclude in Section 6 and give further research directions in Section 7.

2 Background

2.1 Software Transactional Memory

Software Transactional Memory (STM) was introduced by [21] in 1995 as an alternative to lock-based synchronisation in concurrent programming which, in general, is notoriously difficult to get right. This is because reasoning about the interactions of multiple concurrently running threads and low level operational details of synchronisation primitives is *very hard*. The main problems are:

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

Worse, concurrency does not compose. It is very difficult to write two functions (or methods in an object) acting on concurrent data which can be composed into a larger concurrent behaviour. The reason for it is that one has to know about internal details of locking, which breaks encapsulation and makes composition dependent on knowledge about their implementation. Therefore, it is impossible to compose two functions e.g. where one withdraws some amount of money from an account and the other deposits this amount of money into a different account: one ends up with a temporary state where the money is in none of either accounts, creating an inconsistency - a potential source for errors because threads can be rescheduled at any time.

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

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

In the paper [22] the authors use a model of STM to simulate optimistic and pessimistic STM behaviour under various scenarios using the AnyLogic simulation package. They conclude that optimistic STM may lead to 25% less retries of transactions. The authors of [23] analyse several Haskell STM programs with respect to their transactional behaviour. They identified the roll-back rate as one of the key metric which determines the scalability of an application. Although STM might promise better performance, they also warn of the overhead it introduces which could be quite substantial in particular for programs which do not perform much work inside transactions as their commit overhead appears to be high.

2.2 Parallelism, Concurrency and STM in Haskell

In our case studies we are using the functional programming language Haskell. The paper of [14] gives a comprehensive overview over the history of the language, how it developed and its features and is very interesting to read and get accustomed to the background of the language. Note that Haskell is a *lazy* language which means that expressions are only evaluated when they are actually needed.

2.2.1 Side Effects

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

The unique feature of Haskell is that it allows to indicate in the *type* of a function that it does have side effects and what kind of effects they are. There are a broad range of different effect types available, to restrict the possible effects a function can have e.g. drawing random numbers, sharing read/write state between functions, etc. Depending on the type, only specific operations are available, which is then checked by the compiler. This means that a program which tries to read from a file in a function which only allows drawing random numbers will fail to compile.

Here we are only concerned with two effect types: The `IO` effect context can be seen as completely unrestricted as the main entry point of each Haskell program runs in the `IO` context which means that this is the most general and powerful one. It allows all kind of input/output (IO) related side effects: reading/writing a file, creating threads, write to the standard output, read from the keyboard, opening network connections, mutable references, etc. Also the `IO` context provides functionality for concurrent locks and global shared references. The other effect context we are concerned with is `STM` and indicates the STM context of a function - we discuss it more in detail below.

A function with a given effect type needs to be executed with a given effect runner which takes all necessary parameters depending on the effect and runs a given effectful function returning its return value and depending on the effect also an effect related result. Note that we cannot call functions of different effect types from a function with another effect type, which would violate the guarantees. A function without any side effect is called *pure*. Calling a *pure* function though is always allowed because it has, by definition, no side effects.

Although such a type system might seem very restrictive at first, we get a number of benefits from making the type of effects we can use explicit. First we can restrict the side effects a function can have to a very specific type which is guaranteed at compile time. This means we can have much stronger guarantees about our program and the absence of potential run time errors. Second, by the use of effect runners, we can execute effectful functions in a very controlled way, by making the effect context explicit in the parameters to the effect runner.

2.2.2 Parallelism & Concurrency

Haskell makes a very clear distinction between parallelism and concurrency. Parallelism is always deterministic and thus pure without side effects because although parallel code can be run concurrently, it does by definition not interact with data of other threads. This can be indicated through types: we can run pure functions in parallel because for them it doesn't matter in which order they are executed, the result will always be the same due to the concept of referential transparency.

Concurrency on the other hand is potentially nondeterministic because of nondeterministic interactions of concurrently running threads through shared data. Although data in functional programming is immutable, Haskell provides primitives which allow to share immutable data between threads. Accessing these primitives is only possible from within an `IO` or `STM` context (see below) which means that when we are using concurrency in our program, the types of our functions change from pure to either a `IO` or `STM` effect context.

Note that spawning tens of thousands or even millions of threads in Haskell is no problem, because threads in Haskell have a *very* low memory footprint due to being lightweight user space threads, also known as green threads, managed by the Haskell Runtime System, which maps them to physical operating system worker threads [24].

2.2.3 STM

The work of [25, 26] added STM to Haskell which was one of the first programming languages to incorporate STM into its main core and added the ability to composable operations. There exist various implementations of STM in other languages as well (Python, Java, C#, C/C++, etc) but we argue, that it is in Haskell with its type system and the way how side effects are treated where it truly shines.

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

Thus the ability to *restart* a block of actions without any visible effects is only possible due to the nature of Haskells type system: by restricting the effects to `STM` only, prevents uncontrolled effects which cannot be rolled back.

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

- `TVar` A transactional variable which can be read and written arbitrarily;
- `TArray` A transactional array where each cell is an individual shared data, allowing much finer grained transactions instead of e.g. having the whole array in a `TVar`;
- `TChan` A transactional channel, representing an unbounded FIFO channel;
- `TMVar` A transactional *synchronising* variable which is either empty or full. To read from an empty or write to a full `TMVar` will cause the current thread to block and retry its transaction when the `TMVar` was updated by another thread.

2.2.4 An example

We provide a short example to demonstrate the use of STM. To show the retry semantics more clearly, we use `STM` within a `StateT` effect context. A `StateT` effect allows to read and write some state, which in this example we simply set to be an `Int` value. The example code takes a transactional variable `TVar` which holds an `Int` and runs within a `StateT` effect, providing read and write access to an `Int`, and an `STM` effect returning an `Int`:

```
stmAction :: TVar Int -> StateT Int STM Int
stmAction v = do
  -- print a debug output and increment the value in StateT
  Debug.trace "increment!" (modify (+1))
  -- read from the TVar
  n <- lift (readTVar v)
  -- await a condition: content of the TVar >= 42
  if n < 42
    -- condition not met, therefore retry: block this thread
    -- until the TVar v is written by another thread, then
```

```
    -- try again
    then lift retry
    -- condition met: return content ot TVar
    else return n
```

When `stmAction` is run, it prints an `'increment!'` debug message to the console and increments the value in the `StateT`. Then it awaits a condition for as long as `TVar` is less then 42 the action will retry whenever it is run. If the condition is met, it will return the content of the `TVar`. To run `stmAction` we need to spawn a thread:

```
stmThread :: TVar Int -> IO ()
stmThread v = do
  -- the initial state of the StateT effect
  let s = 0
  -- run the state with initial value of s (0)
  let ret = runStateT (stmAction v) s
  -- atomically run the STM action
  (a, s') <- atomically ret
  -- print final result
  putStrLn("final StateT state     = " ++ show s' ++
           ", STM computation result = " ++ show a)
```

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

```
main :: IO ()
main = do
  -- create a new TVar with initial value of 0
  v <- newTVarIO 0
  -- start the stmThread and pass the TVar
  forkIO (stmThread v)
  -- do 42 times...
  forM_ [1..42] (\i -> do
    -- use delay to 'make sure' that a retry is happening for every increment
    threadDelay 10000
    -- write new value to TVar using atomically, will cause the STM
    -- thread to wake up and retry
    atomically (writeTVar v i))
```

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

3 STM in ABS

In this section we give a short overview of how to apply STM in ABS. We fundamentally follow a time-driven approach in both case studies where the simulation is advanced by some given Δt and in each step all agents are executed. To employ parallelism, each agent runs within its own thread and agents are executed in lock-step, synchronising between each Δt which is controlled by the main thread. This way of stepping the simulation is introduced in [27] on a conceptual level, where the authors name it *concurrent update-strategy*. See Figure 1 for a visualisation of our concurrent, time-driven lock-step approach.

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

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

3.1 Adding STM to agents

A detailed discussion of how to add STM to agents on a technical level is beyond the focus of this paper as it would require to give an in-depth technical explanation of how our agents are actually implemented [19].

However, the concepts are similar to the example in Section 2.2.4. The agent behaviour is an `STM` action and has access to the environment either through a `TVar` or `TArray` and performs read and write operations directly on it. Each agent itself is run within its own thread, and synchronises with the main thread. Thus, it takes

Haskells MVar synchronisation primitives to synchronise with the main thread and simply runs the STM agent behaviour each time it receives the next tick DTime:

```
agentThread :: RandomGen g
            => Int            -- Number of steps to compute
            -> SIRAgent g     -- Agent behaviour
            -> g              -- Random-number generator of the agent
            -> MVar SIRState  -- Synchronisation back to main thread
            -> MVar DTime     -- Receiving DTime for next tick
            -> IO ()
agentThread 0 _ _ _ _ = return () -- all steps computed, terminate thread
agentThread n agent rng retVar dtVar = do
  -- wait for dt to compute current step
  dt <- takeMVar dtVar
  -- compute output of current step
  let agentSTMAction = runAgent agent
  -- run the agents STM action atomically within IO
  ((ret, agent'), rng') <- atomically agentSTMAction
  -- post result to main thread
  putMVar retVar ret
  -- tail recursion to next step
  agentThread (n - 1) agent' rng retVar dtVar
```

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

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

4 Case Study 1: Spatial SIR Model

Our first case study is the SIR model which is a very well studied and understood compartment model from epidemiology [28], which allows to simulate the dynamics of an infectious disease like influenza, tuberculosis, chicken pox, rubella and measles spreading through a population [29].

In it, 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 β other people per time unit and become infected with a given probability γ when interacting with an infected person. When infected, a person recovers *on average* after δ time units and is then immune to further infections. An interaction between infected persons does not lead to re-infection, thus these interactions are ignored in this model.

We followed in our agent-based implementation of the SIR model the work [18] but extended it by placing the agents on a discrete 2D grid using a Moore (8 surrounding cells) neighbourhood [19]. A visualisation can be seen in Figure 2.

Due to the continuous-time nature of the SIR model, our implementation follows the time driven [30] approach. This requires us to sample the system with very small Δt, which means that we have comparatively few writes to the shared environment which will become important when discussing the performance results.

4.1 Experiment Design

In this case study we compare the performance of three implementations under varying numbers of CPU cores and agent numbers. The code of all implementations can be accessed freely from the repository [31].

1. Sequential - This is the original implementation as discussed in [19] where the discrete 2D grid is shared amongst all agents as read-only data and the agents are executed sequentially within the main thread without any concurrency.
2. STM - This is the same implementation as the *Sequential* but agents run now in the `STM` context and have access to the discrete 2D grid through a transactional variable `TVar`. This means that the agents now communicate indirectly by reads and writes through the `TVar`.
3. Lock-Based - This is exactly the same implementation as the *STM* one, but instead of running in the `STM` context, the agents now run in the `IO` context. They share the discrete 2D grid using a reference and have access to a lock to synchronise access to the reference.

Each experiment was run until $t = 100$ and stepped using $\Delta t = 0.1$. For each experiment we conducted 8 runs on our machine (see Table 1) under no additional

OS	Fedora 28 64-bit
RAM	16 GByte
CPU	Intel Quad Core i5-4670K @ 3.4GHz (4th Gen.)
HD	250Gbyte SSD
Haskell	GHC 8.2.2
Java	OpenJDK 1.8.0

Table 1: Machine and Software Specs for all experiments

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

Table 2: SIR performance comparisons on 51x51 (2,601 agents) grid with varying number of cores. Timings in seconds (lower is better).

workload and report the mean. Further, we checked the visual outputs and the dynamics and they look qualitatively the same as the reference *Sequential* implementation [19]. A rigorous comparison of all three implementations is beyond the focus of this paper but we refer to the use of property-based testing, as shown in [32]. In the experiments we varied the number of agents (grid size) as well as the number of cores when running concurrently - the numbers are always indicated clearly.

4.2 Constant Grid Size, Varying Cores

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

Comparing the performance and scaling to multiple cores of the *STM* and *Lock-Based* implementations shows that the *STM* implementation significantly outperforms the *Lock-Based* one and scales better to multiple cores. The *Lock-Based* implementation performs best with 3 cores and shows slightly worse performance on 4 cores as can be seen in Figure 3. This is no surprise because the more cores are running at the same time, the more contention for the lock, thus the more likely

Grid Size	STM	Lock-Based (4 cores)	Lock-Based (3 cores)
51 x 51 (2,601)	**20.2**	41.9	38.6
101 x 101 (1,0201)	**74.5**	170.5	171.6
151 x 151 (22,801)	**168.5**	376.9	404.1
201 x 201 (40,401)	**302.4**	672.0	720.6
251 x 251 (63,001)	**495.7**	1,027.3	1,117.2

Table 3: Performance comparison of *STM* and *Lock-Based* SIR implementations on varying grid sizes. Timings in seconds (lower is better).

Grid Size	Commits	Retries	Ratio
51 x 51 (2601)	2601000	1306.5	0.0
101 x 101 (10201)	10201000	3712.5	0.0
151 x 151 (22801)	22801000	8189.5	0.0
201 x 201 (40401)	40401000	13285.0	0.0
251 x 251 (63001)	63001000	21217.0	0.0

Table 4: Retry ratios of the SIR *STM* implementation on varying grid sizes on 4 cores.

synchronisation happening, resulting in higher potential for reduced performance. This is not an issue in *STM* because no locks are taken in advance.

4.3 Varying Grid Size, Constat Cores

In this experiment we varied the grid size and used constantly 4 cores. Because in the previous experiment *Lock-Based* performed best on 3 cores, we additionally ran Lock-Based on 3 cores as well. The results are reported in Table 3 and plotted in Figure 4.

It is clear that the *STM* implementation outperforms the *Lock-Based* implementation by a substantial factor. Surprisingly, the *Lock-Based* implementation on 4 core scales just slightly better with increasing agents number than on 3 cores, something we wouldn't have anticipated based on the results seen in Table 2.

4.4 Retries

Of very much interest when using STM is the retry ratio, which obviously depends highly on the read-write patterns of the respective model. We used the stm-stats [33] library to record statistics of commits, retries and the ratio. The results are reported in Table 4.

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

Table 5: SIR *STM* performance on 16 and 32 cores on Amazon EC2. Timings in seconds (lower is better).

Independent of the number of agents we always have a retry ratio of 0.0. This indicates that this model is *very* well suited to STM, which is also directly reflected in the much better performance over the *Lock-Based* implementation. Obviously this ratio stems from the fact, that in our implementation we have *very* few writes, which happen only in case when an agent changes from *Susceptible* to *Infected* or from *Infected* to *Recovered*.

4.5 Going Large-Scale

To test how far we can scale up the number of cores in both the *Lock-Based* and *STM* cases, we ran two experiments, 51x51 and 251x251, on Amazon EC instances with a larger number of cores than our local machinery, starting with 16 and 32 to see if we are running into decreasing returns. The results are reported in Table 5.

As expected, the *Lock-Based* approach doesn't scale up to many cores because each additional core brings more contention to the lock, resulting in an even more decreased performance. This is particularly obvious in the 251x251 experiment because of the much larger number of concurrent agents. The *STM* approach returns better performance on 16 cores but fails to scale further up to 32 where the performance drops below the one with 16 cores. In both STM cases we measured a retry ratio of 0, thus we conclude that with 32 cores we become limited by the overhead of STM transactions [23] because the workload of an STM action in our SIR implementation is quite small.

4.6 Discussion

The timing measurements speak a clear language. Running in `STM` and sharing state using a transactional variable `TVar` is much more time efficient than both the *Sequential* and *Lock-Based* approach. On 4 cores *STM* achieves a speedup factor of 3.6, nearly reaching the theoretical limit. Obviously both *STM* and *Lock-*

Based sacrifice determinism, which means that repeated runs might not lead to same dynamics despite same initial conditions. Still, by sticking to STM, we get the guarantee that the source of this nondeterminism is concurrency within the `STM` context but *nothing else*. This we can not guarantee in the case of the *Lock-Based* approach as all bets are off when running within the `IO` context. The fact to have *both* the better performance *and* the stronger static guarantees in the *STM* approach makes it *very* compelling.

5 Case Study 2: SugarScape

One of the first models in Agent-Based Simulation was the seminal Sugarscape model developed by Epstein and Axtell in 1996 [20]. Their aim was to *grow* an artificial society by simulation and connect observations in their simulation to phenomenon observed in real-world societies. In this model a population of agents move around in a discrete 2D environment, where sugar grows, and interact with each other and the environment in many different ways. The main features of this model are (amongst others): searching, harvesting and consuming of resources, wealth and age distributions, population dynamics under sexual reproduction, cultural processes and transmission, combat and assimilation, bilateral decentralized trading (bartering) between agents with endogenous demand and supply, disease processes transmission and immunology.

We implemented the *Carrying Capacity* (p. 30) section of Chapter II of the book [20]. There, in each step agents search (move) to the cell with the most sugar they see within their vision, harvest all of it from the environment and consume sugar based on their metabolism. Sugar regrows in the environment over time. Only one agent can occupy a cell at a time. Agents don't age and cannot die from age. If agents run out of sugar due to their metabolism, they die from starvation and are removed from the simulation. The authors report that the initial number of agents quickly drops and stabilises around a level depending on the model parameters. This is in accordance with our results as we show in Figure 5 and guarantees that we don't run out of agents. The model parameters are as follows:

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

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

5.1 Experiment Design

We compare four different implementations with the code freely accessible from the repository [34]:

1 Sequential - All agents are run after another (including the environment) and the environment is shared amongst the agents using a read and write state context.

2 Lock-Based - All agents are run concurrently and the environment is shared using a global reference amongst the agents which acquire and release a lock when accessing it.

3 STM TVar - All agents are run concurrently and the environment is shared using a `TVar` amongst the agents.

4 STM TArray - All agents are run concurrently and the environment is shared using a `TArray` amongst the agents.

Ordering The model specification requires to shuffle agents before every step ([20], footnote 12 on page 26). In the *Sequential* approach we do this explicitly but in the *Lock-Based* and both *STM* approaches we assume this to happen automatically due to race conditions in concurrency, thus we arrive at an effectively shuffled processing of agents because we implicitly assume that the order of the agents is *effectively* random in every step. The important difference between the two approaches is that in the *Sequential* approach we have full control over this randomness but in the *STM* and *Lock-Based* not. This has the consequence that repeated runs with the same initial conditions might lead to slightly different results. This decision leaves the execution order of the agents ultimately to Haskell's Runtime System and the underlying operating system. We are aware that by doing this, we make assumptions that the threads run uniformly distributed (fair) but such assumptions should not be made in concurrent programming. As a result we can expect this fact to produces non-uniform distributions of agent runs but we assumed that for this model this does not has a significance influence. In case of doubt, we could resort to shuffling the agents before running them in every step. This problem, where also the influence of nondeterministic ordering on the correctness and results of ABS has to be analysed, deserves in-depth research on its own. Again we refer to the technique of property-based testing as shown in [32] as this issue is beyond the focus of this paper.

Note that in the concurrent implementations we have two options for running the environment: either asynchronously as a concurrent agent at the same time with the population agents or synchronously after all agents have run. We must be careful though as running the environment as a concurrent agent can be seen as conceptually wrong because the time when the regrowth of the sugar happens is now completely random. In this case it could happen that sugar regrows in the very first transaction or in the very last, different in each step, which can be seen as a violation of the model specifications. Thus we do not run the environment concurrently with the agents but synchronously after all agents have run.

We follow [35] and measure the average number of steps per second of the simulation over 60 seconds. For each experiment we conducted 8 runs on our machine (see Table 1) under no additional workload and report the average. In the experiments we varied the number of cores when running concurrently - the numbers are always indicated clearly.

5.2 Constant Agent Size

In a first approach we compare the performance of all implementations on varying numbers of cores. The results are reported in Table 6 and plotted in Figure 6.

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

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

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

Table 6: Comparison of steps per seconds (higher is better) and retries (lower is better) of various Sugarscape implementations with constant agent numbers. Using 50x50 grid with 500 initial agents on varying cores.

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

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

5.3 Scaling up Agents

So far we kept the initial number of agents at 500, which due to the model specification, quickly drops and stabilises around 200 due to the carrying capacity of the environment as described in the book [20] section *Carrying Capacity* (p. 30).

We now measure the performance of our approaches under increased number of agents. For this we slightly change the implementation: always when an agent dies it

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

Table 7: Steps per second (higher is better) of various Sugarscape implementations with varying agent numbers. Using 50x50 grid with varying number of agents with 4 (and 3) cores except the *Sequential* (1 core) implementation.

spawns a new one which is inspired by the ageing and birthing feature of Chapter III in the book [20]. This ensures that we keep the number of agents roughly constant (still fluctuates but doesn't drop to low levels) over the whole duration. This ensures a constant load of concurrent agents interacting with each other and demonstrates also the ability to terminate and fork threads dynamically during the simulation.

Except for the *Sequential* approach we ran all experiments with 4 cores (*TVar* with 3 as well). We looked into the performance of 500, 1,000, 1,500, 2,000 and 2,500 (maximum possible capacity of the 50x50 environment). The results are reported in Table 7 and plotted in Figure 7.

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

What seems to be very surprising is that in the *Sequential* and *TVar* cases the performance with 2,500 agents is *better* than the one with 2,000 agents. The reason for this is that in the case of 2,500 agents, an agent can't move anywhere because all cells are already occupied. In this case the agent won't rank the cells in order of their payoff (max sugar) to move to but just stays where it is. We hypothesize that due to Haskells laziness the agents actually never look at the content of the cells in this case but only the number which means that the cells themselves are never evaluated which further increases performance. This leads to the better performance in case of *Sequential* and *TVar* because both exploit laziness. In the case of the *Lock-Based*

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

Table 8: Sugarscape *STM* performance on 16 and 32 cores on Amazon EC2. Values are steps per second (higher is better). Retry ratio in brackets.

approach we still arrive at a lower performance because the limiting factor are the unconditional locks. In the case of the *TArray* approach we also arrive at a lower performance because it seems that STM perform reads on the neighbouring cells which are not subject to lazy evaluation.

We also measured the average retries both for *TVar* and *TArray* under 2,500 agents where the *TArray* approach shows best scaling performance with 0.01 retries whereas *TVar* averages at 3.28 retries. Again this can be attributed to the better transactional data structure which reduces retry ratio substantially to near-zero levels.

5.4 Going Large-Scale

To test how far we can scale up the number of cores in both the *Lock-Based* and *TArray* cases, we ran the two experiments (carrying capacity and rebirthing) on Amazon EC instances with increasing number of cores starting with 16 and 32 to see if we run into decreasing returns. The results are reported in Table 8.

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

5.5 Comparison with other approaches

The paper [35] reports a performance of 17 steps in RePast, 18 steps in MASON (both non-parallel) and 2,000 steps per second on a GPU on a 128x128 grid. Although our *Sequential* implementation, which runs non-parallel as well, outperforms the RePast and MASON implementations of [35], one must be very well aware that these results were generated in 2008, on current hardware of that time.

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

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

5.6 Discussion

This case study showed clearly that besides being substantially faster than the *Sequential* implementation, *STM* implementations are also able to perform considerably better than a *Lock-Based* approach even in the case of the Sugarscape model which has a much higher complexity in agent behaviour and dramatically increased number of writes to the environment.

Further, this case study demonstrated that the selection of the right transactional data structure is of fundamental importance when using STM. Selecting the right transactional data structure is highly model-specific and can lead to dramatically different performance results. In this case study the *TArray* performed best due to many writes but in the SIR case study a *TVar* showed good enough results due to the very low number of writes. When not carefully selecting the right transactional data structure which supports fine-grained concurrency, a lock-based implementation might perform as well or even outperform the STM approach as can be seen when using the `TVar`.

Although the `TArray` is the better transactional data structure overall, it might come with an overhead, performing worse on low number of cores than a `TVar` approach but has the benefit of quickly scaling up to multiple cores. Depending on the transactional data structure, scaling up to multiple cores hits a limit at some point. In the case of the `TVar` the best performance is reached with 3 cores. With the `TArray` we reached this limit around 16 cores.

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

6 Conclusion

In this paper we investigated the potential for using STM for parallel, large scale ABS and come to the conclusion that it is indeed a very promising alternative over lock-based approaches as our case studies have shown. The STM implementations all consistently outperformed the lock-based ones and scaled much better to larger number of CPUs. Besides, the concurrency abstractions of STM are very powerful, yet simple enough to allow convenient implementation of concurrent agents without the problems of lock-based implementation. Due to most ABS being primarily pure computations, which do not need interactive input from the user, files or network during simulation, the fact that no such interactions can occur within an agent when running within STM is not a problem.

Further, STM primitives map nicely to ABS concepts. When having a shared environment, it is natural either using `TVar` or `TArray`, depending on the environments nature. Also, there exists the `TChan` primitive, which can be seen as a persistent message box for agents, underlining the message-oriented approach found in many agent-based models [36, 37]. Also `TChan` offers a broadcast transactional channel, which supports broadcasting to listeners which maps nicely to a proactive environment or a central auctioneer upon which agents need to synchronize. The benefits of these natural mappings are that using STM takes a big portion of burden from the modeller as one can think in STM primitives instead of low level locks and concurrent operational details.

The strong static type system of Haskell adds another benefit. By running in the `STM` instead of `IO` context makes the concurrent nature more explicit and at the same time restricts it to purely STM behaviour. So despite obviously losing the reproducibility property due to concurrency, we still can guarantee that the agents can't do arbitrary IO as they are restricted to STM operations only.

Depending on the nature of the transactions, retries could become a bottle neck, resulting in a live lock in extreme cases. The central problem of STM is to keep the retries low, which is directly influenced by the read/writes on the STM primitives. By choosing more fine-grained and suitable data structures e.g. using a `TArray` instead of an indexed array within a `TVar`, one can reduce retries and increase performance significantly and avoid the problem of live locks as we have shown.

Despite the indisputable benefits of using STM within a pure functional setting like Haskell, it exists also in other imperative languages (Python, Java and C++, etc) and we hope that our research sparks interest in the use of STM in ABS in general and that other researchers pick up the idea and apply it to the established imperative languages Python, Java, C++ in the ABS community as well.

7 Further Research

So far we only implemented a tiny bit of the Sugarscape model and left out the later chapters which are more involved as they incorporate direct synchronous communication between agents. Such mechanisms are very difficult to approach in GPU based approaches [35] but should be quite straightforward in STM using `TChan` and retries. However, we have yet to prove how to implement reliable synchronous agent interactions without deadlocks in STM. It might be very well the case that a truly concurrent approach is doomed due to the following [38] (Chapter 10. Software Transactional Memory, *What Can We Not Do with STM?*): *"In general, the class of operations that STM cannot express are those that involve multi-way communication between threads. The simplest example is a synchronous channel, in which both the reader and the writer must be present simultaneously for the operation to go ahead. We cannot implement this in STM, at least compositionally [..]: the operations need to block and have a visible effect — advertise that there is a blocked thread — simultaneously."*.

A drawback of STM is that it is not fair because *all* threads, which block on a transactional primitive, have to be woken up upon a change of the primitive, thus a FIFO guarantee cannot be given. We hypothesise that for most models, where the STM approach is applicable, this has no qualitative influence on the dynamics as agents are assumed to act conceptually at the same time and no fairness is needed. We leave the test of this hypothesis for future research. This is connected to our assumption that concurrent execution has no qualitative influence on the dynamics. Although repeated runs with same initial conditions might lead to different results due to nondeterminism, the dynamics follow still the same distribution as the one from the sequential implementation. To verify this we can make use the techniques of property-based testing as shown in [32] but we leave it for further research.

Declarations

Availability of data and materials

The datasets used and/or analysed during the current study are available from the corresponding author on reasonable request.

Competing interests

The authors declare that they have no competing interests.

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Authors' contributions

JT initiated the idea and the research, did the implementation, experiments, performance measurements, and writing. POS supervised the work, gave feedback and supported the writing process. All authors read and approved the final manuscript.

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Figures

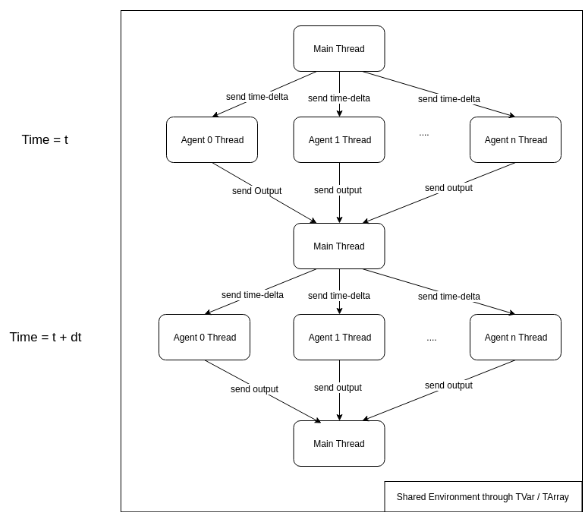


Figure 1: Diagram of the parallel time-driven lock-step approach.

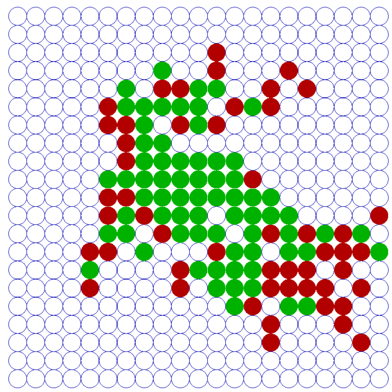


Figure 2: Simulating the spatial SIR model with a Moore neighbourhood, a single infected agent at the center, contact rate $\beta = \frac{1}{5}$, infection probability $\gamma = 0.05$ and illness duration $\delta = 15$. Infected agents are indicated by red circles, recovered agents by green ones. The susceptible agents are rendered as blue hollow circles for better contrast.

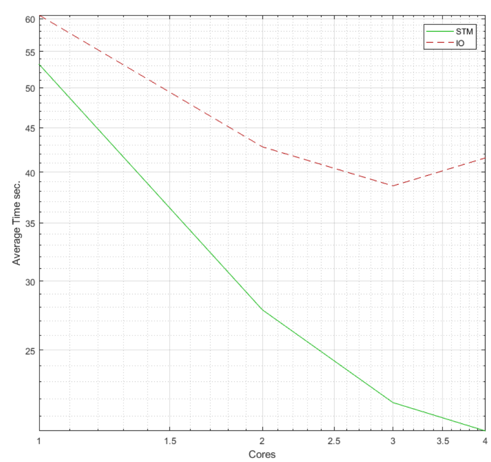


Figure 3: Performance and scaling comparison of *STM* and *Lock-Based* SIR implementations on multiple cores. Note that the Lock-Based implementation performs worse on 4 than on 3 cores due to lock contention.

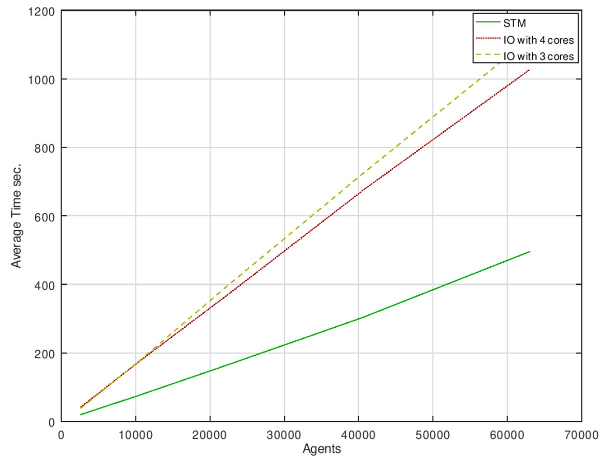
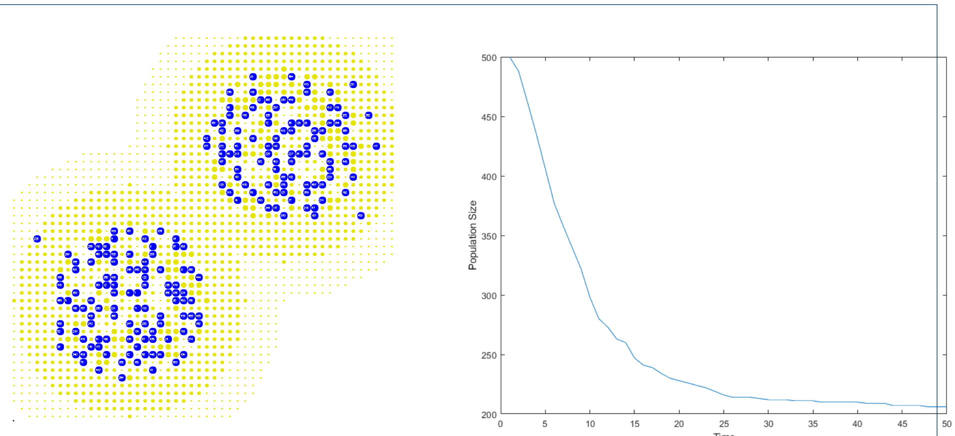


Figure 4: Performance comparison of *STM* and *Lock-Based* SIR implementations on varying grid sizes.



(a) Visualisation of the Sugarscape at $t = 50$

(b) Dynamics population size over 50 steps

Figure 5: Visualisation of our SugarScape implementation and dynamics of the population size over 50 steps. The white numbers in the blue agent circles are the agents unique ids.

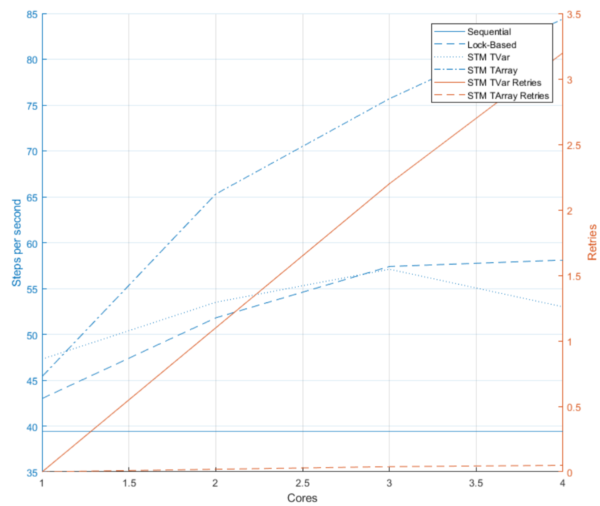


Figure 6: Comparison of steps per seconds (higher is better) and retries of various Sugarscape implementations with constant agent numbers. Using a 50x50 grid and 500 initial agents on varying cores.

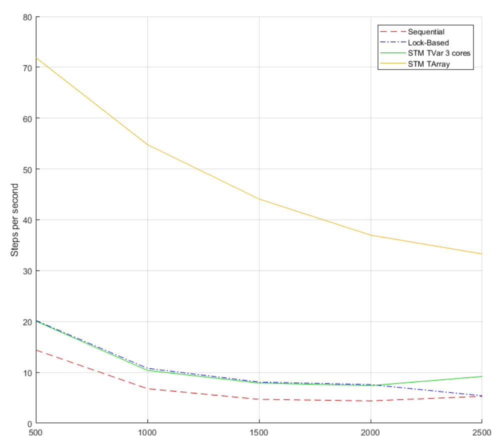


Figure 7: Steps per second (higher is better) of various Sugarscape implementations with varying agent numbers. Using 50x50 grid and varying number of agents with 4 (and 3) cores except the *Sequential* (1 core) implementation.