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Spatial Effects in Stochastic Microscopic Models - Case Study and Analysis

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Abstract: In this paper we are going to present techniques to investigate the theoretical background of so called microscopic models (i.e. models consisting of a large number of individual but yet cooperating actors). We will lay special emphasis on the analysis of so called aggregated numbers, hereby speaking of usually scalar, summarising variables, dependent on all actors simultaneously, which are typically some kind of sums or statistics. We are going to analyse the behaviour of those quantities in case of a very large number, respectively in the limit case, an infinite number of individual actors. We will especially focus on the influence of spatial relationships between the actors on the aggregated number. Stochastic methods are going to play the key role in this theory. Furthermore we will apply the results of the theoretical research on three different microscopic models, each of them chosen to particularly point onto an important observation. The first model, a simplified epidemics model, is going validate the theory and demonstrates how to use it. The second model, based on famous *Game of Life* by John H. Conway, will reveal the limits of the method and finally, the third model, an extension of the second one, will show the benefits and applicability of the analytically derived theory.

Keywords: Microscopic Modelling, Agent-Based Modelling, Diffusion Approximation, Mean-field Approximation, Aggregation, Markov-Process

1. INTRODUCTION

The term *microscopic*, often used by modelling experts to communicated a basic idea about a certain model is, almost independent of the scientific research field, usually associated with a *lot* of individual actors or particles (inter)acting in a certain environment. Any further interpretation is difficult and might be misleading as there is no global definition of the term *microscopic* respectively *microscopic model* all scientific fields agree with. E.g. physicists might receive motivation developing microscopic models by needs of spatial discretisation of a liquid via simple particles (Chen and Doolen (1998)), whereas computer engineers might be motivated by simulating highly complex behaving human (Bruckner et al. (2012)).

In context of our work we will use the term *microscopic* model for dynamic (hereby used to indicate temporal dependent) models, consisting of a high number of similar sub-models, which will furthermore be denoted as *actors*. Hereby the idea of increasing the number of actors has to be possible and meaningful in the specific context. By the term we want to cover big classes of models like e.g. agent-based models, cellular automata or microsimulation models. As a microscopic model does not necessarily contain a spatial structure we will focus on those kind of models. Nevertheless the presented technique can also be applied on models without spatial relationships.

In this paper we will not discuss different motivations and applications of microscopic models, but are going to present a technique to investigate the theoretical background of microscopic models. We will lay special emphasis on the analysis of so called aggregated numbers, typically some kind of sums or statistics. We are going to analyse the behaviour of those quantities in case of a very large number, respectively in the limit case, an infinite number of individual actors. We will especially focus on the influence of spatial relationships between the actors on the aggregated number. Furthermore we will apply the results of the theoretical research on three different microscopic models, each of them chosen to particularly point onto an important observation.

2. ANALYTICAL METHODS

As a part of the complex-systems-theory (see Wolfram (1988)) the analysis of microscopic models, especially those in which actors depend on each other during runtime, is generally motivated by possible emergence of unexpected and sometimes even chaotic effects. Hereby unexpected describes the necessity to simulate the whole model in order to make any prognosis for the simulation-output at all. This is different e.g. for differential equation models for which a steady state analysis can be performed. It is not surprising that it is hardly possible to predict the behaviour of a single sample actor as it is dependent on the behaviour of all or at least some other individuals

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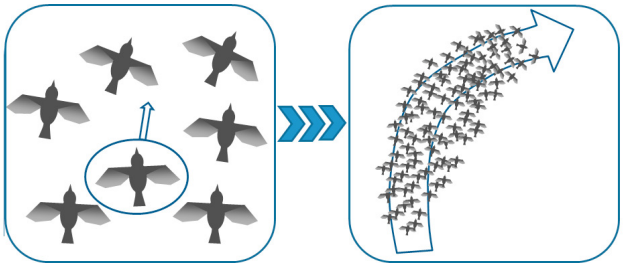

Fig. 1. Unexpected emergent behaviour of the mass on the example of a bird flock. Simple individual rules lead to complex unpredictable behaviour of the flock.

too. However it is surprising that it is also very difficult to predict the behaviour of the whole crowd respectively so called aggregated numbers of the model (see Figure 1). This effect can be seen as a special kind of swarm-intelligence.

2.1 Aggregated Numbers

Aggregated numbers in microscopic models are summaries of the state of all individual actors and are used to describe the overall state of the model. As already mentioned they are sometimes simple statistics of the actors like mean or variance of the individual states. We furthermore define that a function a is called *aggregation function* of a microscopic model consisting of m_i, $i = 1 \dots N$ actors with corresponding states $\vec{s}_i \in \Gamma$ if it fulfils the following properties:

(1) $a : \prod_{i=1}^{N} \Gamma \to K \subseteq \mathbb{R}^d$, $(\vec{s_1}, \dots, \vec{s_N}) \mapsto a(\vec{s_1}, \dots, \vec{s_N})$
(2) K is independent of N and compact
(3) $a(p(\vec{s_1}, \dots, \vec{s_1})) = a(\vec{s_1}, \dots, \vec{s_1})$ for all permutations p

Property (2) guarantees that the function-output is qualitatively independent of the number of actors. Especially $a(\vec{s_1}, \dots, \vec{s_N})$ remains finite if $N \to \infty$. Property (3) provides that all actors are treated the same way and no index is preferred. Outputs of this function are finally called aggregated numbers. As the states $s_i(t)$ are time-dependent so is usually $a(t)$. Of all aggregation functions surely the empiric mean and the empiric variance are the best known. Here we want to introduce a slight adaptation of the empiric mean which will furthermore pose the basis for analytic research. The aggregation function

$$o_k(\vec{s_1}, \dots, \vec{s_N}) := \frac{1}{N} \sum_{i=1}^{N} \mathbb{I}_k(s_i), \tag{1}$$

with the indicator function $\mathbb{I}_k(x) = \delta_{k,x}$, will be called *counting function* of the state k as is counts the fraction of all actors currently sharing this state. The output of this function is furthermore called *counting variable* or *counting vector* and can be calculated for all possible states k of the actors. If the number of possible states is discrete, the counting variables fulfil $\sum_k o_k = 1$.
To understand the following chapters it is crucial to notice that we hereby projected a system consisting of N actors, each having one of d different states at a time, onto a system consisting of d different state variables, each taking values between zero and one (see Figure 2).

Target of the following sub-section is the prediction of the temporal development of the counting function for

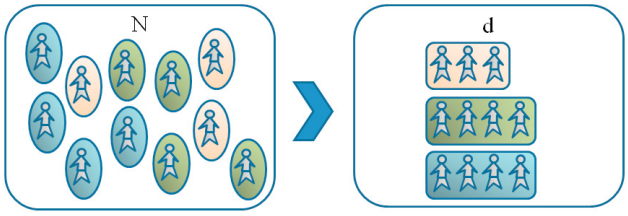

Fig. 2. Graphical interpretation of the principle of the counting function defined in (1).

simplified stochastic microscopic models without directly performing the simulation. As the model is meant to be stochastic also the counting function is a stochastic variable. Hence we will derive formulas for mean and variance of the function.

2.2 Diffusion Approximation

Diffusion approximation of Van Kampen (see Kampen (2007) and Kampen, N. G. van (1982)) respectively at least its results are, by knowledge of the author, still core of all theorems developed to perform aggregated analysis of microscopic models - so called mean-field theorems (some examples: Boudec et al. (2007), Benoit et al. (2006)). Although the same theorems can also be derived by other approaches (like e.g. Itô-calculus) too, we will present the diffusion-approximation method, because knowledge about extended stochastic calculus is not required in order to understand it. Basically the idea was developed to investigate probability-densities of quantum mechanical particles and was reworked and extended several times to enlarge its field of application.

Roots of this method lie within Markov-Theory and, to be more precise, within the Kolmogorow Equation (see Kolmogorov, A (1931)) respectively the discrete part of its differential form, the Master Equation: Given a regular, time continuous and homogeneous Markov process $X(t)$ which only takes discrete values in Ω the following equation holds for its probability function:

$$\frac{\partial P(x,t)}{\partial t} = \sum_{y \in \Omega} P(y,t)\omega_{x,y} - P(x,t)\omega_{y,x}. \tag{2}$$

Hereby $\omega_{x,y}$ are called transition-rates of the Markov process and can be seen as time-derivatives of transition-probabilities. For the derivation of this equation we refer to Gardiner (2009). As discrete, finite state-spaces Γ (compare with the definition of aggregated numbers) is most applicable for the desired test cases we furthermore only consider these, which are furthermore denoted with $\{1, \dots, d\}$.

The main idea of diffusion-approximation respectively mean-field approximation, is to use this equation to express the temporary behaviour of the counting-function as defined in (1). This approach only works correctly if the counting-function itself is a Markov-process. To analyse under which circumstances this feature is given was key objective of this work. The most valuable observation hereby is that the actors itself do *not* necessarily need to be Markov-processes in order to inherit the Markov-property to the counting variables. It is sufficient that the transition probabilities of the individual actors can be written as

$$P(s_i(t+h) = x | s_i(t) = y_i, \vec{o}(t) = \vec{k}). \quad (3)$$

I.e. the probability for a state change of actor i may not only depend on the former state of the actor itself, but also on the former state of the counting variables. Obviously this is a big relaxation to the claim that all actors need to be individual Markov-processes to be suitable for the theory. Yet all actors need to act *memoryless*. For the proof of this observation we refer to Bicher (2013).

Although this observation finally allows to treat microscopic models wherein actors change their states stochastically dependent on each other, it is not trivial to determine under which circumstances a given model is suitable for the analysis. Typically microscopic models are defined via individual rules including movement rules (e.g. on a lattice), contacts, neighbourhood (respectively contact ranges), transition rates based on individual contacts or similar features. Many of these rules can be simplified so that finally transitions only depend on counting variables. Examples are given in chapter 3.

2.3 Resulting Equations and Error Boundaries

In case the basically stochastic actors fulfil (3), the probability function of the counting variable satisfies master-equation (2) and is suitable for diffusion approximation. Hereby the strategy of M. Aoki (Aoki (2002)) was used which was refined on the one hand for time-discrete (i.e. models with constant time-steps) models and on the other hand for $|\Gamma| > 2$ in Bicher (2013). The results are based on the knowledge of the following state dependent transition probabilities of the counting vector o:

$$\omega_{\vec{k}, \vec{k} + \frac{1}{N}(\vec{e_i} - \vec{e_j})} := P\left(o_i(t+h) = k_i + \frac{1}{N}, o_j(t+h) = k_j - \frac{1}{N} | \vec{o}(t) = \vec{k} \right). \quad (4)$$

The vectors $\vec{e}_i$ are usually called unit vectors and fulfil $e_i = (\delta_{i,j})_{j=1}^{d}$. Hereby the expression in the second line denotes the probability that one of the actors formerly in state j changed into state i during this time-step which increases element i of the counting vector by N^{-1} and equally decreases element j. As a matter of volume only the results of the analytic transformations including Taylor-expansion and an Itô-motivated-substitution can be shown here. We refer to Aoki (2002) or Bicher (2013) for detailed derivation. With errors qualitatively depending on inverse powers of $\sqrt{N}$ the mean $\vec{\phi}(t)$ of the counting variable $\vec{o}(t)$ fulfils

$$\frac{d\vec{\phi}}{dt} = \sum_{i \neq j} (\vec{e_i} - \vec{e_j}) \omega_{\vec{\phi}, \vec{\phi} + \frac{1}{N}(\vec{e_i} - \vec{e_j})}, \ \vec{\phi}(0) = \vec{o}(0). \quad (5)$$

According to literature (de Aguiar et al. (2003)) this equation is sometimes called mean-field theorem. As a direct implication of the additionally derived Fokker-Planck equation for the density $P(t,x)$ of the counting-variable given in (6), the corresponding variance can be seen to converge towards zero if $N \to \infty$ also with inverse orders of $\sqrt{N}$. This observation shows that the counting variable looses its fluctuations for a high number of actors, which can be seen as a sort of *law of large numbers*.

$$\frac{\partial \Pi}{\partial t} = \Pi f(\vec{\phi}, \vec{\xi}(t)) + \nabla_{\xi(t)} \Pi \cdot \vec{F}(\vec{\phi}) + g(H_{\xi(t)} \Pi, \vec{\phi})$$
$$\Pi(t, \vec{\xi}(t)) := P(t, \sqrt{N}(\vec{o}(t) - \vec{\phi}(t)), \ \Pi(0, \vec{\xi}) = \delta_0(\vec{\xi}) \quad (6)$$

Symbols ∇ and H in (6) denote nabla and hessian differential operator and δ, appearing in the initial condition, denotes a delta-distribution. As the spatial integral over the density has to remain constant we have homogeneous Neumann-boundaries outside of $\times_{i=1}^{d}[-\phi_i(t), 1 - \phi_i(t)]$ providing conservation of total-probability [1].

Although equations (5) and (6) appear very unhandy in the first place, they can usually be simplified and solved numerically. In several cases (6) can analytically be solved by a multivariate Gaussian curve affirming the close relationships to the *law of large numbers*. Equation (5) is a usually non-linear ordinary differential equation with $\frac{d}{dt}\left(\sum_{i=1}^{d} \phi_i(t)\right) = 0$.

As a matter of the attempt to approximate system variables of usually time discrete (clocked) microscopic systems with time continuous differential equations some additional - i.e. in addition to errors dependent inversely on the number of actors - discretisation [2] errors between the moments of the microscopic system and the solutions of equations (5) and (6) have to be accepted [3]. The time-continuous transition-rates necessary for the diffusion-approximation have to be approximated with simple transition probabilities. Basically this can be seen as a sort of reverted explicit Euler (respectively Euler-Maruyama see Kloeden (1999)) strategy. Calculations made in Bicher (2013) proved quantitative error boundaries mainly dependent on the size of the transition probabilities (4) and their gradients. Especially a temporal scaling in combination with an equal scaling of the probabilities and, of course, $N \to \infty$ leads to convergence.

3. CASE STUDIES

The following three simple test cases are used to show how the presented technique can be applied to especially calculate means of counting variables for very simplified toy-models. The three cases are chosen properly to draw attention onto three different issues. A simple agent-based model based on a SIR strategy (see section 3.1) will be used for a direct verification of the mean-equation (5) and how the equation can be derived for a concrete application. A cellular automaton (CA) based on John H. Conways Game of Life (see section 3.2) furthermore shows that the technique can fail occasionally. A modification of the CA (see section 3.3) finally helps to understand the value of the theoretical analysis as a steady-state analysis of equation (5) needs to be performed.

3.1 SIR - Model

Susceptible-Infected-Recovered, short S-I-R, donates a modelling strategy to simulate the trend of a simple epidemic. Hereby each individual can solely have one of the

[1] This interval can be verified as $o_i \in [0,1]$ and $\xi_i = \sqrt{N}(o_i - \phi_i)$

[2] Rather "inverse-discretisation" or "continuisation"

[3] Diffusion-approximation is basically limited to time-continuous Markov-processes.

three aforementioned states which can only be passed through in this specific order: susceptible, respectively healthy, individuals might get infected and finally either die or become recovered and therefore immune against the disease. Based on this strategy a lot of both simplified, as well as very successful, validated models were developed during the last decades. We want to lay emphasis on a simple agent-based model developed in order to support lectures for modelling and simulation at the Vienna University of Technology:

Initially a number of N individuals is randomly placed on a rectangular lattice with $M >> N$ cells. Based on whether there is an infected agent in one of three specific neighboured cells of a susceptible one, the healthy agent has a certain probability α to get infected too. Infected agents themselves have a certain probability β to recover each time-step. At the end of each time-step a movement-function, inspired by classical Lattice-Gas Celluar-Automata for the simulation of fluids (see Chen and Doolen (1998)), allows all agents to receive a new position on the lattice and hence also new neighbours. We will furthermore use the isomorph representation $\Gamma := \{1, 2, 3\} := \{\text{susceptible}, \text{infected}, \text{recovered}\}$ for each agent's state space.

Especially the probability of a single agent to change its state from healthy to infected is difficult to treat as it depends on certain individual agents in the neighbourhood. Yet, globally seen, the corresponding parameter $\omega_{\vec{k},\vec{k}+\frac{1}{N}(\vec{e}_2-\vec{e}_1)}$, which denotes the rate for an increase of the second line of the counting variable by N^{-1}, respectively the rate for one healthy agent to get infected, can be calculated and seen only to depend on the counting variable itself. A closer look at the definition on the model shows that the rate, furthermore called *infection rate*, can be split up into three parts:

$$\omega_{\vec{k},\vec{k}+\frac{1}{N}(\vec{e}_2-\vec{e}_1)} = u \cdot v \cdot \alpha. \tag{7}$$

Hereby α donates the aforementioned infection probability. Rate u donates the rate to receive a healthy agent if an agent is targeted and corresponds to the fraction of agents sharing this state respectively $\vec{o}_1$. Rate v donates the probability that at least one infected agent is placed next to the susceptible one. As the carrier of the disease can be placed at one of three possible neighboured cells this, introducing a population density $\rho := \frac{\text{number of agents}}{\text{number of cells}}$, can be approximated by

$$v \approx 3 \cdot \frac{\text{number of infected agents}}{\text{number of cells}} = 3\vec{o}_2\rho. \tag{8}$$

Success of this approximation lies within two important aspects:

- Rate, respectively probability, for a "healthy" agent to meet an "infected" one during a time-step can be calculated with binomial-distribution arguments to $1-(1-\vec{o}_2\delta)^3$. The density needs to be small enough to justify the simplification $1-(1-\vec{o}_2\delta)^3 \approx 3\vec{o}_2\delta$.
- The movement rules consider good mixture among the agents and the size and number of clusters does not increase if the number of agents N is raised. Case study number two will show how drastically different movement rules can influence aggregated results.

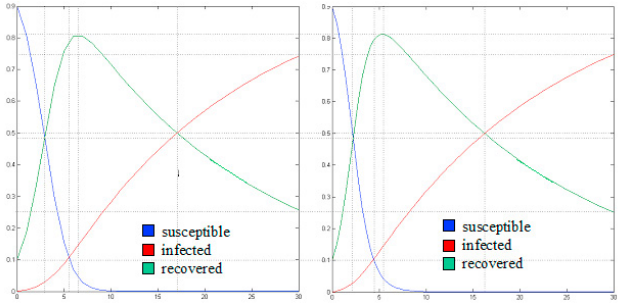

Fig. 3. Comparison of results of the agent-based model with its mean-field approximation, the famous SIR equations.

Both features are provided for the parameter-sets chosen for this case study. Finally we achieve the rates given in (9) and, as all other rates vanish, derive the mean-field approximation (10).

$$\begin{aligned} \omega_{\vec{k},\vec{k}+\frac{1}{N}(\vec{e}_2-\vec{e}_1)} &= \vec{o}_1\vec{o}_2 3\rho\alpha \\ \omega_{\vec{k},\vec{k}+\frac{1}{N}(\vec{e}_3-\vec{e}_2)} &= \vec{o}_2\beta \end{aligned} \tag{9}$$

$$\begin{pmatrix} \vec{o}_1 \\ \vec{o}_2 \\ \vec{o}_3 \end{pmatrix}' = \begin{pmatrix} -\vec{o}_1\vec{o}_2 3\rho\alpha \\ \vec{o}_1\vec{o}_2 3\rho\alpha - \vec{o}_2\beta \\ \vec{o}_2\beta \end{pmatrix} \tag{10}$$

This non-linear ordinary differential equation unmasks itself as the famous S-I-R equation derived by Kermack and McKendrick in the early stages of the 20th century (see Kermack and McKendrick (1927)). The success of the diffusion approximation can be seen in Figure 3 and is also documented in Miksch et al. (2013). For a more detailed derivation of the equations for this specific application of the diffusion approximation we refer to Bicher (2013) respectively Bicher and Popper (2013).

In summary, we have observed that the described technique works for this specific case and that necessary rates can be derived by binomial-distribution arguments.

3.2 Classical Game of Life

As already mentioned the derivation of the diffusion-approximation in the first case study relied on the great mixture among the agents granted by their movement rules. To show how badly the strategy can fail otherwise a second example will be presented in form of a cellular automaton (CA). For more informations about CAs we refer to Schneckenreither (2014).

Hereby we want to take an unusual look at John H. Conway's so called Game of Life (Berlekamp (2001)). The very simple, but yet fascinating automaton, is defined by a rectangular lattice and two possible cellular states: $\Gamma := \{1, 2\} \cong \{\text{dead}, \text{alive}\}$.

During a single time-step each "living" cell remains in its state if the number of "living" cells in its Moore-neighbourhood [4] equals two or three, otherwise the cell "dies". A "dead" cell is brought back to live if the number of living cells in its Moore-neighbourhood equals exactly

[4] Moore neighbourhood of a cell denotes eight specific cells: all four direct neighbours as well as all four diagonal neighbours.

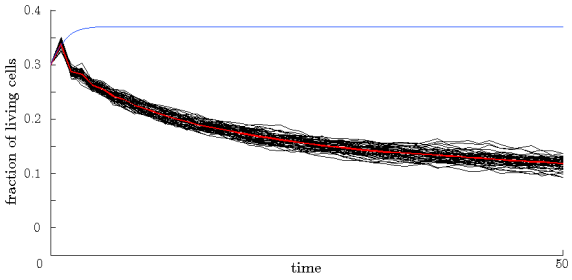

Fig. 4. Some sample simulations of the aggregated Game of Life (black) with estimated mean (red) compared to the numerically determined results of equation (12) (blue).

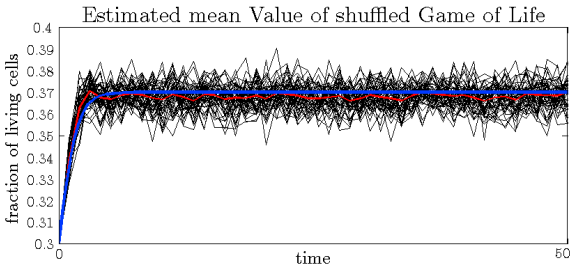

Fig. 5. Some sample simulations of the aggregated Shuffled Game of Life (black) with estimated mean (red) compared to the numerically determined results of equation (12) (blue). We see the success of the shuffling process.

three. All cells are updated simultaneously and the next time-step starts.

Although the majority of its fame comes from the discovery of very interesting spatial patterns we furthermore want to observe Game of Life from an aggregated point of view. We think of the automaton to pose for a kind of population model and argue that each living cell denotes an individual. Therefore we are interested in the temporal development of the overall population density, which, defining N as the number of cells in the observed rectangle, is nothing more than the already defined counting variable of the system wherein each cell poses for one actor.

Similar to the SIR model we try to perform the diffusion-approximation and try to calculate the two corresponding rates. Again we try to derive these with arguments based on binomial-distribution and receive (11) and hence (12).

$$\begin{aligned} \omega_{\vec{k},\vec{k}+N^{-1}(-1,1)^T} &= \binom{8}{3} \vec{o}_1^{\,3} \vec{o}_2^{\,6} \\ \omega_{\vec{k},\vec{k}+N^{-1}(1,-1)^T} &= 1 - \binom{8}{3} \vec{o}_1^{\,4} \vec{o}_2^{\,5} - \binom{8}{2} \vec{o}_1^{\,3} \vec{o}_2^{\,6} \end{aligned} \tag{11}$$

$$\begin{pmatrix} \vec{o}_1 \\ \vec{o}_2 \end{pmatrix}' = \begin{pmatrix} 1 - \binom{8}{3} \vec{o}_1^{\,4} \vec{o}_2^{\,5} - \binom{8}{2} \vec{o}_1^{\,3} \vec{o}_2^{\,6} - \binom{8}{3} \vec{o}_1^{\,3} \vec{o}_2^{\,6} \\ -1 + \binom{8}{3} \vec{o}_1^{\,4} \vec{o}_2^{\,5} + \binom{8}{2} \vec{o}_1^{\,3} \vec{o}_2^{\,6} + \binom{8}{3} \vec{o}_1^{\,3} \vec{o}_2^{\,6} \end{pmatrix} \tag{12}$$

We receive a highly non-linear system of differential equations which can be solved with numerical methods. As the second line of the counting variable is simply one minus the first one it will not be considered in future.

Figure 4 shows that the derived mean field approximation fails in this example after an initial percentage of living cells were initially distributed randomly among the lattice. This is due to the fact that each cell's neighbourhood remains the same for the whole simulation and clustering plays a key role in this model. This observation is affirmed when investigating the curve for the first two or three time steps in which the mean field approximation qualitatively still matches the empiric mean of the aggregated cellular automaton curves before it suddenly drops towards a possible steady state. In summary, we see that movement respectively rearrangement of cells leading to new contacts is an important feature to guarantee that binomial-distribution arguments can be used to calculate the necessary rates for the diffusion-approximation. Without sufficient mixture the presented technique to derive the rates does not work.

3.3 Shuffled Game of Life

In order to see whether it is true that the failure of the strategy use before is due to missing rearrangement of the cells we slightly adapt the cellular automaton by inserting a completely random permutation of all cells at the end of each time-step. We will furthermore denote this model as *Shuffled Game of Life*.

Figure 5 shows some simulation runs and their mean value compared to a numeric solution of (12). Hereby the same initial conditions as in Figure 4 were used. We see that the mean-field approximation works for the shuffled version of the model and how much difference spatial rearrangement can have on the aggregated numbers. We carried on with the study of the model and discovered that some experiments with different initial conditions (i.e. different fractions of initially living cells) lead to very interesting and in the first place unexplainable results. Surprisingly the Monte-Carlo study of these specific simulation runs did not deliver reliable results as the variance between the simulation runs did not seem to converge towards zero. One of these studies can be seen in Figure 6. Reason for this behaviour could be found analysing each simulation run on its own. About a third of the simulation runs delivered an increasing aggregated number converging to an upper bound and two thirds of the simulation runs resulted in a decrease to a lower bound. Performing a Monte Carlo analysis for these kind of simulations is dangerous and fails as the achieved mean value does never express the qualitative behaviour of any simulation run at all (left hand side of Figure 7).

Clarity about these unusually sensitive simulation result is finally gained investigating the derived mean-field approximation (12). Analysis of the differential equation resulted in a detracting steady state very close to the used initial conditions (at about 0.19). Therefore almost insignificant fluctuations at the beginning of the microscopic simulation can invoke that the simulation results either increase towards the upper bound or decrease towards the lower one. Steady state analysis of the equation can be seen graphically at the right hand side of Figure 7.

In summary, diffusion-approximation hereby proved its worth as it not only helped to explain strange simulation

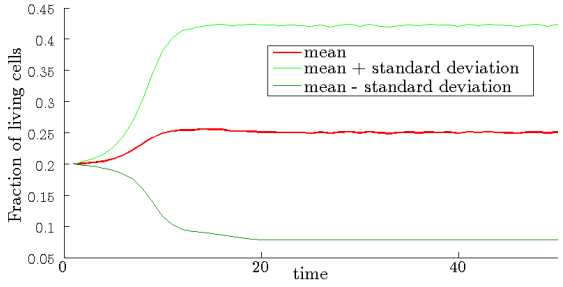

Fig. 6. Monte Carlo analysis of a number of simulation runs for a specific initial condition. Unusually high standard deviations can be observed.

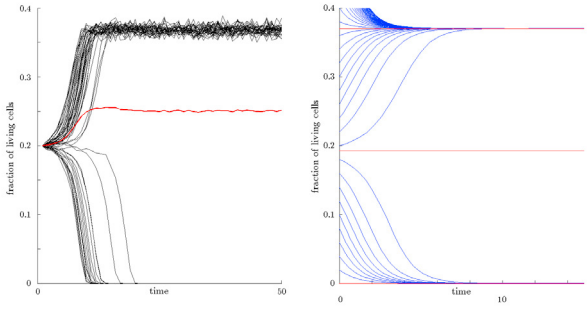

Fig. 7. Left: Sample simulation runs of Shuffled Game of Life for specific initial condition including mean value. Right: Steady state analysis of (12).

results, but also to understand that Monte Carlo analysis can not be used in this specific case. Thus it can be used to understand a given microscopic system and to determine parameter sensitivities without performing millions of simulation runs.

4. CONCLUSION

We presented a technique which can help to contribute to the analysis of microscopic system and based on three simple models proved its validity, its limits, as well as its possible applications. Each of these three properties leave space for further research. As well as using the method to analyse "real" parametrised models, generalisation of the technique is planned in order to cover a bigger bandwidth of microscopic simulation methods.

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