

Methods for Cellular Automata and Evolution Systems in Modelling and Simulation

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Abstract: Cellular automata provide an interesting concept for modelling and simulation. Besides advanced modelling approaches like the Lattice Boltzmann Method cellular automata are also used for simulation in population dynamics, reaction diffusion systems or bio-medicine. While the basic concepts of cellular automata are rather clear and unambiguous, there exists no general mathematical formalism as there is for other modelling approaches like differential equations or stochastic processes. Often such systems are not even labelled as *cellular automata* due to the historic and diverse connotation of this term. This modelling approach is however only applicable for systems that exhibit a certain topological structure. We interpret the topological concepts of such systems as graphs and vector spaces in order to provide a suitable mathematical framework for analysis. Furthermore a generalisation leads to evolution systems (strongly continuous semigroups, abstract Cauchy problems) on the one hand and stochastic processes on the other. This provides access to a variety of mathematical tools and methods for analysing and validating cellular automaton modelling approaches.

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1. INTRODUCTION

1.1 Cellular Automata as a Method for Modelling and Simulation

Cellular automata are in many occasions (e.g. Wolfram (2002)) perceived and treated as *natural systems* consisting of a grid of cells with locally characterised dynamic behaviour. A partially different perception regards cellular automata as a method for modelling and simulation. Of course in both cases the basic ideas and the structure are mostly identical. In the latter case the conception of cellular automata is however used to depict a natural system as an abstract conceptual model and to describe the simplified system in a mathematical fashion (Tab. 1). Also the term *cellular automaton* itself is controversial in this case (a different and more suitable naming is still missing for this contribution).

natural system
abstract conceptual model
mathematical description
implementation on computer system
simulation

Table 1. Simplified modelling process (compare Balci (2012)).

A basic necessity for cellular automata as a viable approach for modelling and simulation is a common under-

standing of the underlying concepts (like cells, states or update rules). In literature (Ganguly et al. (2003); Wolf-Gladrow (2000); ...) the perception of cellular automata is mostly consistent and only varies on a rather high level of detail (p.e. discrete or continuous states). However there exists no agreement on a systematic mathematical formalism, which makes communication unnecessarily complicated and hinders the development of mathematical methods for analysis and model validation.

1.2 Basic Concepts of Cellular Automata

As mentioned before, a cellular automaton is composed of a multitude of equal identifiable cells. These cells are completely passive in the sense that a cell is not aware of its surroundings – like it is possible for agent-based models – but only a container for a state. Each cell takes a state from a set of possible states. The state of a cell changes according to the state of a set of cells called its *neighbourhood*, which may also include the actual cell itself. These state-changes are performed according to an update rule, which is applied on all cells or more precisely their neighbourhoods simultaneously. All simultaneous state changes can be accumulated in an (abstract) evolution operator, which accordingly iterates the states of all cells.

The cells of a cellular automaton either represent a discretised (spatial) domain or represent abstract entities, which are aligned in a regular fashion. Especially in the context

of modelling this differentiation cannot be neglected. Since for every cell a certain set of cells is used to calculate a new state, the resulting network structure of neighbourhood relations is a further important characteristic of cellular automata.

1.3 Definition of Cellular Automata

We propose the following simplified definition of cellular automata (Schneckenreither (2014)):

- (M) a finite set of abstract cells M
- (\mathcal{N}) a neighbourhood mapping $\mathcal{N} : M \rightarrow M^k$
- (\mathbb{S}) a set of possible states \mathbb{S} such that the *global* state of the cellular automaton can be represented as a mapping $\mathcal{S} : M \rightarrow \mathbb{S}$ or $\mathcal{S} \subseteq \mathbb{S}^M$
- (\mathcal{F}) an update function $\mathcal{F} : \mathbb{S}^k \rightarrow \mathbb{S}$

The iteration ($t \in T$) of global states can formally be written as an evolution operator

$$\mathcal{E} : \mathbb{S} \rightarrow \mathbb{S} : \mathcal{S}_t \mapsto \mathcal{S}_{t+1} = \mathcal{F} \circ \mathcal{S}_t \circ \mathcal{N}. \quad (1)$$

This is however only the basic structure of a cellular automaton.

1.4 Topology of Cellular Automata

Usually the cells are aligned in a regular grid like structure. This can be achieved on a mathematical level by introducing a bijective mapping between an index set in \mathbb{Z}^d and the set of cells M as depicted in Fig. 1 or by regarding the set $V := M - M$ as an affine vector space (module). In the first case we call the identification of cells and indices in \mathbb{Z}^d *indexing* or *index mapping* and talk of *ordinary* cellular automata.

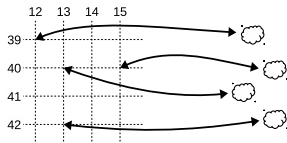


Fig. 1. Regularly arranged cells, Index Mapping.

We may however also allow generalisations and simplifications of the basic concept of ordinary cellular automata for example by regarding an unaligned set of cells which delivers a more abstract conception of cellular automata.

A second *topological* feature of cellular automata is the use of neighbourhoods (\mathcal{N}) as a basis for the calculation and iteration of states. Under the condition that the cells are aligned – either by an index mapping or through a vector space interpretation – this mapping can be synthesised as

$$\mathcal{N} : m \mapsto i \mapsto (i + j_1, \dots, i + j_k) \mapsto (n_1, \dots, n_k) \quad (2)$$

or

$$\mathcal{N} : m \mapsto m + (v_1, \dots, v_k). \quad (3)$$

If there exists no alignment of the cells this mapping must be defined explicitly and can be interpreted as a graphical structure (compare Fig. 2)

$$G = (M, E), \quad E = \bigcup_{m \in M} \{(n, m) : n \in \mathcal{N}(m)\}. \quad (4)$$

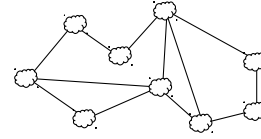


Fig. 2. Graphical representation of the neighbourhood structure.

Since the set of cells M is finite, we have to deal with so-called *boundary conditions* if the cells are arranged in a grid like fashion. Boundary conditions arise when a cell located near the boundary of the grid lacks one or more of its neighbours. We talk of *degraded* neighbourhoods and the update function has to be modified according to the structure of the degradation. This is however not one of the main interests for this contribution.

2. MATHEMATICAL DESCRIPTION OF THE TOPOLOGY OF CELLULAR AUTOMATA

2.1 Graph Theory

As usual for graphs, also the graphical structure of a cellular automaton (i.e. the second topological feature) can be represented using the concept of adjacency matrices. Every vertex (cell) must be identified with a basis vector from $\{0, 1\}^{|M|}$ – from $\mathbb{N}^{|M|}$ etc. for weighted graphs – which yields a one-dimensional indexing $M \rightarrow \{1, \dots, |M|\}$ for the cells such that the matrix $A = (a_{ij})_{i,j \in \{1, \dots, |M|\}}$ defines the edges (neighbourhood relations) of the graph:

$$m_i \in \mathcal{N}(m_j) \iff e_i A e_j = a_{ij} > 0 \quad (5)$$

Since for ordinary cellular automata we already have an indexing $M \rightarrow \mathbb{Z}^d$ in this case the concept of an adjacency matrix can be extended to *adjacency tensors*

$$A : \mathbb{Z}^d \times \mathbb{Z}^d \rightarrow \{0, 1\} : (m_i, m_j) \mapsto A(i, j) = a_{ij} \quad (6)$$

indicating whether m_i is a neighbour of m_j or not.

For ordinary cellular automata the adjacency tensor features a very specific structure. Obviously an adjacency tensor is sparsely occupied. Furthermore due to the fact that the neighbourhoods are defined through a tuple (j_1, \dots, j_k) (compare (2)), the adjacency tensor has band structure and is regular (i.e. every column and row contains the same elements, this corresponds to the regularity of the graph, compare Knauer (2011)) for symmetric neighbourhood relations (i.e. $n \in \mathcal{N}(m) \iff m \in \mathcal{N}(n)$). In Fig. 3 a regular adjacency matrix with band structure is shown.

2.2 Vectorspace Interpretation

Often spatial models incorporate a vector field on M . For example the Lattice Boltzmann Model describes the distribution of velocities for every location on a domain. In this case every neighbour of a cell is associated with a certain velocity vector.

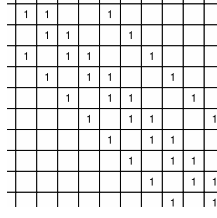


Fig. 3. Adjacency matrix of a cellular automaton. At the boundary of a lattice neighbourhoods can be degraded.

The hexagonal grid for Lattice Gas Cellular Automata is motivated by the isotropy of the lattice tensors. In fact a higher symmetry of the lattice allows more accurate results.

A vectorspace interpretation of the set of cells is also very useful for the transition from discrete sets to continuous domains.

3. EVOLUTION SYSTEMS

A more abstract approach to cellular automata can be formalised in a functional analytic way (Schneckenreither (2014)).

Let M be a topological vector space and $\mathfrak{S} \subseteq \mathbb{S}^M$ a Banach space. For a subset $N \subset M - M$ the projection operator is written as $\pi_{m+N} : \mathfrak{S} \rightarrow \mathbb{S}^N$ with $\ker \pi_{m+N} \subseteq \mathbb{S}^{M \setminus (m+N)} \subset \mathfrak{S}$ and the embeddings are written as $\iota_m : \mathbb{S} \rightarrow \mathfrak{S}$ with $\text{ran } \iota_m \subseteq \mathbb{S}^{\{m\}} \subset \mathfrak{S}$.

We define linear evolution systems by

- (M) a discrete or continuous domain M in a topological vectorspace
- (\mathbb{S}) a set of possible states \mathbb{S} such that there exists a Banach space $\mathfrak{S} \subseteq \mathbb{S}^M$
- (\mathcal{E}) a strongly continuous semigroup \mathcal{E}_{dt} of bounded linear operators on \mathfrak{S}
- (\mathcal{L}) star-shaped¹ sets $N_{dt} \subset M - M$ and functions $\mathcal{F}_{dt} : \mathbb{S}^{N_{dt}} \rightarrow \mathbb{S}$ such that

$$\mathcal{E} = \sum_{m \in M} \iota_m \circ \mathcal{F} \circ \pi_{m+N_{dt}} \quad (7)$$

and

$$\mathcal{I}_{\mathfrak{S}} = \sum_{m \in M} \iota_m \circ \pi_m. \quad (8)$$

Requirements $(M, \mathbb{S}, \mathcal{E})$ yield a strongly continuous semigroup on \mathfrak{S} . This is the basis for connecting evolution systems with parabolic partial differential equations or abstract evolution equations (Kato (1961); Goldstein (1985); Engel and Nagel (2000); ...).

(\mathcal{L}) transfers the concept of neighbourhoods from cellular automata in a straight forward fashion to strongly continuous semigroups: The domain of M or from another perspective the subspace or components of $\mathfrak{S} \subseteq \mathbb{S}^M$ that actually influence the outcome of \mathcal{E}_{dt} at a certain *location*

¹ For simplicity we only regard star-shaped sets N around 0, which means that for every $n \in N$ the line from n to 0 is completely within N .

m is characterised by the set N_{dt} or by $\mathbb{S}^{m+N_{dt}}$, respectively (compare Fig. 4). In other words (for continuous \mathbb{S} only) if $\mathcal{S} = (s_m)_{m \in M}$ then

$$\frac{\partial \mathcal{E}_{dt} \mathcal{S}(m)}{\partial s_n} = 0 \iff n \notin m + N_{dt}. \quad (9)$$

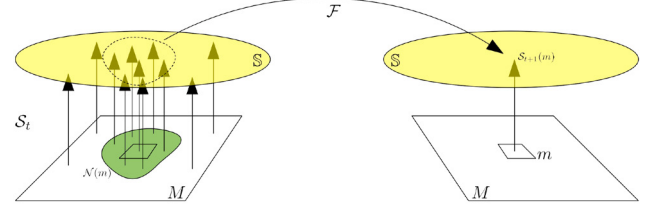


Fig. 4. Local Characterisation. The calculation of a new state depends on a certain subset $\mathcal{N}(m) = m + N$ of the set of cells M .

We call evolution systems satisfying the condition (\mathcal{L}) *locally characterised* evolution systems.

For a discretisation of M into finite components, a locally characterised evolution system corresponds to a cellular automaton. Advanced discretisation methods are for example discussed by Goncalves et al. (2012).

4. LINEAR DISCRETE EVOLUTION SYSTEMS

Discretised linear evolution systems correspond to linear cellular automata. If M is a finite set then \mathbb{S}^M is a finite-dimensional vectorspace and a linear mapping $\mathbb{S}^M \rightarrow \mathbb{S}^M$ can be represented by a matrix $E \in \mathbb{S}^{|M| \times |M|}$ (or by a tensor).

The update function defines a new state as a linear combination of the neighbouring states

$$\mathcal{S}_{t+1}(m) = \sum_{n \in \mathcal{N}(m)} \alpha_{mn} \mathcal{S}_t(n). \quad (10)$$

Usually a cellular automaton features of course a nonlinear evolution operator.

5. INTEGRAL EVOLUTION SYSTEMS

Let us for simplicity assume that \mathcal{E}_{dt} has a representation as an integral operator

$$\mathcal{E}_{dt} \mathcal{S}(m) = \int_{M-M} \kappa_{dt}(v) \mathcal{S}(m+v) dv \quad (11)$$

and that $\mathbb{S} \subseteq \mathbb{R}^p$.

5.1 Local Characterisation

From $\mathcal{E}_{dt} \rightarrow \mathcal{I}_{\mathfrak{S}}$ for $dt \rightarrow 0$ it follows that $\kappa_{dt} \rightarrow \delta_0$. Accordingly the kernels κ_{dt} satisfy the condition

$$\lim_{dt \rightarrow 0} \int_{B_\varepsilon(0)} \kappa_{dt}(v) dv = 1 \quad (12)$$

or in other words for every $\delta > 0$ there exists a $\varepsilon > 0$ such that

$$\left\| \int_{M-M} \kappa_{dt}(v) \mathcal{S}(m+v) dv - \int_{B_\varepsilon(0)} \kappa_{dt}(v) \mathcal{S}(m+v) dv \right\| < \delta \quad (13)$$

for all $\mathcal{S} \in \mathfrak{S}$.

Instead of the ε -ball $B_\varepsilon(0)$ we can also use a star-shaped set $N_{dt} \subset M - M$ such that

$$\left\| \int_{M-M} \kappa_{dt}(v) \mathcal{S}(m+v) dv - \int_{N_{dt}} \kappa_{dt}(v) \mathcal{S}(m+v) dv \right\| < C_{dt}, \quad (14)$$

which means that integral evolution systems can be approximated by locally characterised (integral) evolution systems. In a more abstract fashion this result can be extended to general evolution systems.

5.2 Stochastic Approximation

Let additionally $\kappa_{dt} : M - M \rightarrow \mathbb{R}_+$ be probability densities ($\|\kappa_{dt}\|_1 = 1$) and let $N_{dt} \sim \kappa_{dt}$ be random variables from a probability space $(\Omega, \mathfrak{A}, \mathcal{P})$ to $M - M$.

If v_1, \dots, v_k are realisations of N_{dt} (see Fig. 5), then for growing k according to the law of large numbers,

$$\frac{1}{k} \sum_{i=1}^k \mathcal{S}(m + v_i) \longrightarrow \mathbb{E}[\mathcal{S}(m + N_{dt})]. \quad (15)$$

This allows to approximate integral evolution operators with suitable kernels in a stochastic fashion.

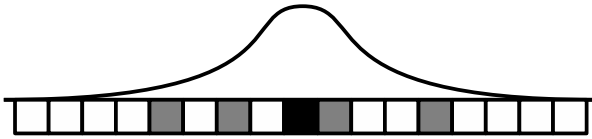


Fig. 5. If κ is a probability density function then the corresponding integral evolution operator in conjunction with the neighbourhood can be approximated stochastically. A random collection of neighbours is chosen accordingly to the distribution implied by κ .

5.3 Example: Gaussian Diffusion

The Gaussian diffusion semigroup is defined through the probability kernels

$$\kappa_{dt}(v) = (4D\pi dt)^{-\frac{d}{2}} \exp\left(-\frac{\|v\|^2}{4Ddt}\right). \quad (16)$$

The corresponding evolution equation is the heat equation

$$\partial_t \mathcal{S} = D \Delta \mathcal{S}. \quad (17)$$

A finite difference discretisation of the heat equation on \mathbb{R}^2 ($d = 2$) yields the following cellular automaton representation:

$$\begin{aligned} (M) \quad & M \subset \mathbb{R}^d \\ (\mathcal{N}) \quad & \mathcal{N} : m \mapsto (m, m + e_1, m + e_2, m - e_1, m - e_2) \\ (\mathbb{S}) \quad & \mathbb{S} = \mathbb{R} \\ (\mathcal{F}) \quad & \mathcal{F} : (s_0, \dots, s_4) \mapsto D \cdot (s_1 + s_2 + s_3 + s_4 - 4s_0) \end{aligned}$$

The discretisation of the integral representation of the Gaussian diffusion semigroup has the form

$$\mathcal{S}_{t+1}(m) = \sum_{v \in \mathbb{R}^2} \hat{\kappa}(v) \mathcal{S}(m+v) \quad (18)$$

where $\hat{\kappa}$ are Bessel functions that can also be calculated from κ by replacing \mathcal{S} in (11) with its Taylor series expansion (which actually yields a partial differential equation).

Since κ_{dt} are probability densities also a stochastic approximation of this system is evident.

6. STOCHASTIC CELLULAR AUTOMATA

In some situations like for example when evolution operators are stochastically approximated, the resulting states are of stochastic character. A mathematical approach to random or stochastic states can happen by representing states as random variables.

Stochastic cellular automata can be defined in the following way, which settles them between Bayesian networks (Friedman et al. (2000)) and multiparameter stochastic processes (Khoshnevisan (2002)).

$$\begin{aligned} (M) \quad & \text{finite set of cells } M \\ (\mathcal{N}) \quad & \text{neighbourhood mapping } \mathcal{N} : M \rightarrow M^k \\ (\mathbb{S}) \quad & \text{separable measurable Hausdorff space } (\mathbb{S}, \mathfrak{B}) \\ & \cdot \text{ random variables } S_{t,m} \text{ from a (Radon-) probability space } (\Omega, \mathfrak{A}, \mathcal{P}) \text{ to } (\mathbb{S}, \mathfrak{B}) \\ (\mathcal{K}) \quad & \text{a Markov-kernel } \mathcal{K} : \mathbb{S}^k \times \mathfrak{B} \rightarrow [0, 1] \\ & \cdot \text{ such that } \mathcal{P}(S_{t+1,m} \in B | S_{t,\mathcal{N}(m)} = \mathbf{s}) = \mathcal{K}(\mathbf{s}, B) \end{aligned}$$

An equivalent definition of stochastic cellular automata can be formulated through filtrations of σ -algebras based on the graphical structure of the neighbourhood relations (Schneckenreither (2014)). Some direct conclusions from stochastic cellular automata include that the global stochastic process, which describes the simultaneous transition of the states of all cells, is a Markov process itself. Furthermore a Chapman-Kolmogorov like equation can be formulated for stochastic cellular automata.

6.1 Simplifications

For application in modelling and simulation a discretisation of \mathbb{S} or a parameter representation of the random states can be used.

We restrict the random states to a certain family of distributions such that $S_{t,m} \sim \text{Dist}_{\theta_{t,m}}$ and every possible random state can be identified with a deterministic parameter θ . The stochastic process can then be described by an iteration of deterministic values

$$\hat{\mathcal{F}} : (\theta_{t,n_1}, \dots, \theta_{t,n_k}) \mapsto \theta_{t+1,m}. \quad (19)$$

For discretised \mathbb{S} , random states can be represented by random vectors \mathbf{p} and we obtain a multilinear mapping

$$\hat{\mathcal{F}} : (\mathbf{p}_{t,n_1}, \dots, \mathbf{p}_{t,n_k}) \mapsto \mathbf{p}_{t+1,m}. \quad (20)$$

As a consequence a stochastic cellular automaton with discrete states can be represented by a transition tensor analogously to transition matrices for Markov chains.

7. APPLICATION EXAMPLE: EPIDEMIC MODEL

The classical SIR-type epidemic model observes a homogeneous population which is categorised into susceptible (S), infected (I) and recovered (R) individuals. Infections are based on the contact behaviour of susceptible and infected individuals. In a homogeneous population the contact rate is given by SI . Let α be the infection rate and β the recovery rate. The following system of ordinary differential equations describes the dynamics of the classical SIR epidemic model:

$$\begin{aligned} S_t &= -\alpha SI \\ I_t &= \alpha SI - \beta I \\ R_t &= \beta I \end{aligned} \quad (21)$$

7.1 Spatial Model

A spatially inhomogeneous population can be modelled by a diffusion process on a two-dimensional domain $\Omega \subset \mathbb{R}^2$ (compare Schneckenreither et al. (2008)). Let S , I and R be the densities $T \times \Omega \rightarrow \mathbb{R}_+$ of the population.

$$\begin{aligned} \partial_t S - D_S \Delta_x S &= -\alpha SI \\ \partial_t I - D_I \Delta_x I &= \alpha SI - \beta I \\ \partial_t R - D_R \Delta_x R &= \beta I \end{aligned} \quad (22)$$

D_S , D_I , D_R are the diffusion coefficients of the three sub-populations.

This system is equivalent to an evolution system of the form

$$\mathcal{E}_{dt}^S S(x) = \int_{\Omega} \kappa_{dt}^S(v) S(x+v) dv - G_{dt}(S(x), I(x)). \quad (23)$$

Obviously κ_{st}^* are Gaussian kernels (16) and this evolution system is locally characterised (see Section 5.1). The corresponding partial differential equation (22) is a semilinear parabolic system. There however also exists a quasilinear model for spatial SIR-type epidemics

$$\begin{aligned} \partial_t S &= -(\alpha I + \gamma \Delta_x I) S \\ \partial_t I &= (\alpha I + \gamma \Delta_x I) S - \beta I \\ \partial_t R &= \beta I \end{aligned} \quad (24)$$

which is equivalent to a locally characterised evolution system of the form

$$\mathcal{E}_{dt}^S S(x) = S(x) - S(x) \int_{\Omega} \kappa_{dt}(v) I(x+v) dv. \quad (25)$$

7.2 Age-Structured Model

A further important demographic parameter in connection with epidemiology is age. An age-structured population was for example investigated by Keyfitz and Keyfitz (1997) or Iannelli and Martcheva (2003) and modelled by the following semilinear partial differential equation where S , I and R as well as $P := S + I + R$ are functions $T \times [0, a_{\max}] \rightarrow \mathbb{R}_+$ where a_{\max} is the maximum age and μ

is the *force of mortality* (or age-dependent natural death-rate).

$$\begin{aligned} \partial_t S - \partial_a S &= -\lambda(t, a) S - \mu(a) S \\ \partial_t I - \partial_a I &= \lambda(t, a) S - \beta(a) I - \mu(a) I \\ \partial_t R - \partial_a R &= \beta(a) I - \mu(a) R \end{aligned} \quad (26)$$

The parameter

$$\lambda(t, a) := \int_0^\infty \kappa(a, s) \frac{I}{P}(t, s) ds \quad (27)$$

depends on the contact behaviour (κ) between different age-groups (a and s) of the population.

The number of (susceptible) newborns can be calculated from $m(a)$, “the probability of a woman of age a giving birth in a unit of time” (Keyfitz and Keyfitz (1997)) $S(0, t) = \int_0^\infty m(a) P(a, t) da$. Or in case of short-time observations by using the current birth rate.

However for real contact data between individuals with specific age the corresponding integral evolution system is not locally characterised, because the typical contact behaviour of a population $\kappa(\cdot, \cdot)$ exhibits a shape as illustrated in Fig. 6 and in particular Fig. 7.

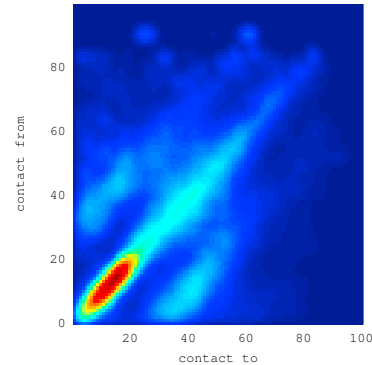


Fig. 6. Contact data from the POLYMOD Project (Mossong et al. (2008)), which was funded by the European Commission (Contract number: SSP22-CT-2004-502084). This figure shows the number of contacts from individuals with a certain age to other individuals with certain age. The significance of contacts between parents and their children is clearly visible.



Fig. 7. Typical form of a contact distribution $\kappa(a, a + \cdot)$, describing the likelihood of interaction of a person aged a to other persons with age in $[a - 100, a + 100]$. This figure only shows the general form of a contact distribution. For example ages below 0 are not possible such that this function is not necessarily symmetric. The peaks at -30 respectively $+30$ indicate the interaction of children with their parents and vice versa (i.e. generations).

Since the contact behaviour is not of local character it cannot be formulated as a differential (of order two) as in Section 7.1. Iannelli and Martcheva (2003) perform an eigenvalue and spectral analysis of the nonlinear semigroup corresponding to (26) in order to determine equilibria and stability of the system.

7.3 Cellular Automaton Approximation

We implement the model described in (26) based on population data of Austria (Statistik Austria (2015)) and contact data from the POLYMOD project (Mossong et al. (2008)) and try to compare experimental results with the analytic findings in (Iannelli and Martcheva (2003)).

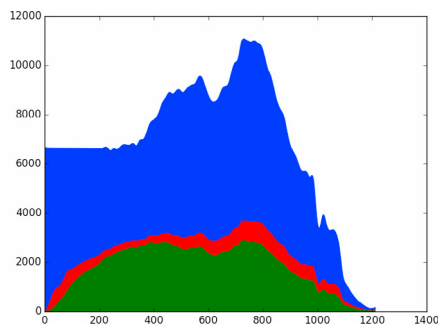


Fig. 8. Screenshot of a simulation of the age-structured SIR model. Age in months is displayed on the horizontal axis. The number of susceptible, infected and recovered are shown in blue, red and green on the vertical axis.

8. CONCLUSION AND OUTLOOK

Like the spatially inhomogeneous SIR model, also the age-structured SIR model allows an additional stochastic formulation. Furthermore a combination of both model approaches could be interesting.

A general investigation of cellular automata in terms of evolution systems (that is semigroup theory, partial differential equations, abstract Cauchy problems, ...), graphs, vectorspaces and stochastic processes promises to provide a lot of direct results which can be transferred from these areas to cellular automata and used in connection with specific applications.

Furthermore we see that cellular automata require a mathematical perspective (for example through evolution systems or semigroups) in order to allow analytic treatment in the first place.

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