A white-box model of population growth

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Background. Integration of reductionist and holistic approaches is one of the great challenges for mathematical modeling. Mathematical models of complex systems are divided into black-box, white-box and grey-box types. A black-box model is completely nonmechanistic as internal mechanisms of a modeled complex system are hidden. A white-box model demonstrates direct mechanisms of functioning of a complex system. It holistically shows all events at microlevel, mesolevel and macrolevel of a modeled system at all stages of its dynamics. Earlier we have used the white-box modeling for verification and reformulation of the competitive exlusion principle. Here we investigate in more details our white-box model of single-species population dynamics. This is fundamentally important because most basic ecological models are of black-box type, including Malthusian, Verhulst, Lotka-Volterra models. **Methods.** Our white-box model of single-species population growth is a purely logical deterministic individual-based cellular automata model. A biological prototype of the model is a vegetative propagation of rhizomatous lawn grasses. Using the Monte Carlo method, we investigate a role of different initial positioning of an individual in the habitat. We also investigate different size and structure of the habitat and two types of fecundity. **Results.** We have created and investigated a logical white-box model of an ecosystem with one species. This model demonstrates mechanisms of the S-shaped and double S-shaped population growth. We have investigated population growth limited by different factors, in particular by resources, habitat structure, intraspecific competition, lifetime of individuals, regeneration time and fecundity of individuals. We have compared the S-shaped curves with J-shaped curves of population growth. **Conclusion.** We present a basic white-box model of population dynamics which combines reductionist and holistic approaches. Integration of reductionist and holistic approaches is provided by the simultaneous modeling of both part-whole and cause-effect relations in complex system. We consider this holystic multi-level white-box modeling approach as a method of artificial intelligence which works as hyper-logical automatic deductive inference that provides direct mechanistic insights into complex systems. The white-box modeling by logical deterministic cellular automata is a perspective way for investigation not only of population dynamics but also of any complex systems.

INTRODUCTION

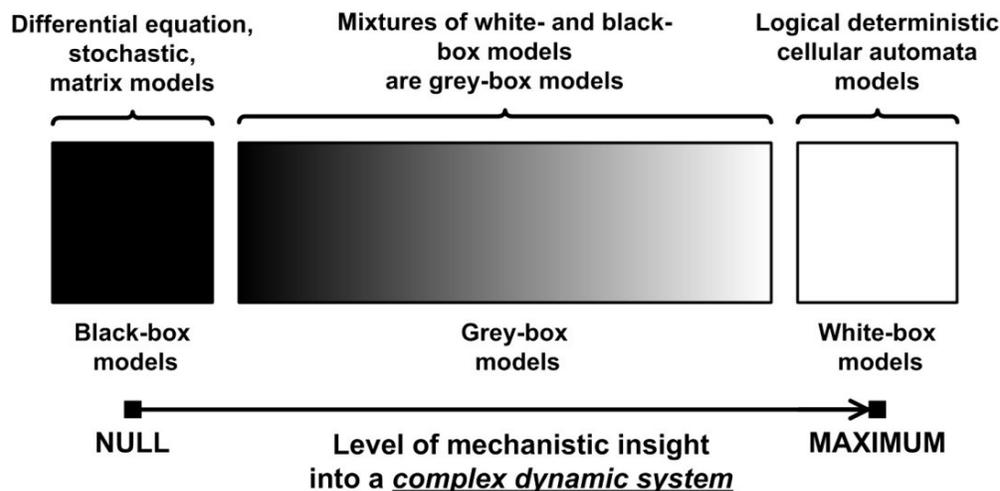
Background

A mechanistic approach corresponds to the classical ideal of science. Existing mathematical approaches to complex systems modeling are rather phenomenological than mechanistic. Mechanicalness in this case assumes integration of reductionist and holistic approaches. David Tilman drew attention to the fact that ecologists investigate interspecific competition phenomenologically, rather than mechanistically (Tilman 1987). The article was published in 1987, however it is relevant for biodiversity science and mathematical modeling of complex systems even today. It discusses a problem among field experiments designed to test for the existence of interspecific competition in natural communities. Tilman suggests, '*The design of the experiments, though, is a memorial to the extent to which the often-criticized Lotka-Volterra competition equations still pervade ecological thought. The experiments used a nonmechanistic, Lotka-Volterra-based, phenomenological definition of competition: two species compete when an increase in the density of one species leads to a decrease in the density of the other, and vice versa. ... With a few notable exceptions, most ecologists have studied competition by asking if an increase in the density of one species leads to a decrease in the density of another, without asking how this might occur. ... Experiments that concentrate on the phenomenon of interspecific interactions, but ignore the underlying mechanisms, are difficult to interpret and thus are of limited usefulness.*'(Tilman 1987)

Without mechanistic models we will not be able to overcome the limitations of phenomenological approach which hides from us internal functional mechanisms of ecosystems. Only a mechanistic approach will allow us not only to constate the loss of biodiversity, but to understand what needs to be done to save it. A mechanistic mathematical model of a complex system should be completely discrete, logical and consisting of cause-effects and of part-whole relations between micro-subsystems, meso-subsystems and a whole macro-system. The purpose of this study is a deeper mechanistic investigation of our logical white-box model of single-species population dynamics, which is an alternative to the Verhulst model of population growth (Kalmykov & Kalmykov 2013; Kalmykov & Kalmykov 2011).

Black-box, grey-box and white-box models

How to create such a mechanistic model? First, we need to know how to mechanistically model a complex dynamic system. A complex dynamic system may be considered as consisting of subsystems that interact. Interactions between subsystems lead to the emergence of new properties, e.g. of a new pattern formation. Therefore we should define these subsystems and logically describe their interactions in order to create and investigate a mechanistic model. If we want to understand how a complex dynamic system works, we must understand cause-effect relations and part-whole relations in this system. The causes should be sufficient to understand

37 their effects and the parts should be sufficient to understand the whole. There are three types of
38 possible models for complex dynamic systems: black-box, grey-box and white-box models (Fig.
39 1).

40 **Figure 1: Three types of mathematical models for complex dynamic systems.** This
41 is a schematic representation of a black-box model, a grey-box model and a white-box
42 model with the level of their mechanistic understanding.

43 Black-box models are completely nonmechanistic. We cannot investigate interactions of
44 subsystems of such a non-transparent model. A white-box model of complex dynamic systems
45 has 'transparent walls' and directly shows underlying mechanisms – all events at micro-, meso-
46 and macro-levels of a modeled dynamic system are directly visible at all stages. Earlier we
47 demonstrated, that the logical deterministic cellular automata approach allows to create white-
48 box models of complex dynamic systems (Kalmykov & Kalmykov 2013). A micro-level is
49 modeled by the lattice sites (cellular automata cells). A meso-level of local interactions of micro-
50 objects is modeled by the cellular automata neighbourhood. A macro-level is modeled by the
51 entire cellular automata lattice. As a rule, this approach is used in 'overloaded' form, what makes
52 it less transparent. This is achieved by adding differential equations and stochasticity. Grey-box
53 models are intermediate and combine black-box and white-box approaches. Basic ecological
54 models are of black-box type, e.g. Malthusian, Verhulst, Lotka-Volterra models. These models are
55 not individual-based and cannot show features of local interactions of individuals of competing
56 species. That is why they principally cannot provide a mechanistic insight into complex dynamic
57 systems`.

58 A white-box model of a complex system is completely mechanistic. A white-box modeling is
59 axiomatic modeling. Before creating a white-box model we need to formulate an intrinsic
60 axiomatic system based on a general physical understanding of the subject area under study.
61 Axioms are the first principles of the subject. When scientists verify a theory first of all they
62 should strictly verify its axioms.

On the white-box modeling of population dynamics

Let's consider an example of the inadequacy of ecological models in result of incompleteness of their axiomatic system. There are many models of population dynamics that do not take into account what happens with individuals after their death. Dead individuals instantly disappear with roots, stubs, etc. '*One reason for the lack of understanding on the part of most botanists results from their failure to take into account the phenomenon of regeneration in plant communities, which was first discussed in general terms by A. S. Watt in 1947.*' (Grubb 1977)

Stephen Hubbell in his Unified Neutral Theory of Biodiversity (UNTB) in fact refuses a mechanistic understanding of interspecific competition: '*We no longer need better theories of species coexistence; we need better theories for species presence-absence, relative abundance and persistence times in communities that can be confronted with real data. In short, it is long past time for us to get over our myopic preoccupation with coexistence*' (Hubbell 2001). However, he admits that '*the real world is not neutral*' (Rosindell et al. 2012). Since the basic postulate (axiom) of the UNTB about ecological neutrality of the presence of similar species in the ecosystem is wrong, this theory cannot be true. In addition, local interactions of individuals are absent in the neutral models in principle. That is why neutral models cannot provide a mechanistic insight into biodiversity. The UNTB models are of black-box and dark grey-box types only – Fig. 1. We agree with James Clark, that the dramatic shift in ecological research to focus on neutrality distracts environmentalists from the study of real biodiversity mechanisms and threats (Clark 2009). Within the last decade, the neutral theory has become a dominant part of biodiversity science, emerging as one of the concepts most often tested with field data and evaluated with models (Clark 2009). Neutralists are focused on considering unclear points of the neutral theory – the ecological drift, the link between pattern and process, relations of simplicity and complexity in modeling, the role of stochasticity and others, but not the real biodiversity problems themselves (Rosindell et al. 2012). Attempts to understand neutrality instead of biodiversity understanding look like attempts to explain the obscure by the more obscure. Nonmechanistic ecological models make it difficult to answer basic questions, e.g. Why are there so many closely allied species? (Anonymous 1944) An example of the difficult ecological discussion is the debates 'Ecological neutral theory: useful model or statement of ignorance?' on the forum Cell Press Discussions (Craze 2012).Understanding of mechanisms of interspecific coexistence is a global research priority. These mechanisms can allow us to efficiently operate in the field of biodiversity conservation. Obviously, such knowledge must be based on mechanistic models of species coexistence. Unfortunately, ecological modelers prefer to use the heaviest black-box mathematical methods, which cannot produce mechanistic models of complex dynamic systems in principle, and not use simple and long-known purely logical deterministic cellular automata, which easily can produce white-box models and directly obtain clear mechanistic insights into dynamics of complex systems.

Here, as a simple example, we show our white-box model of population and ecosystem dynamics (Fig. 2) and characterise this cellular automata model. We investigate in details an ecosystem model with one species. This model is both the simplest and most basic, because it demonstrates not only the well known phenomenological S-shaped population growth curve, but also the

104 underlined individual-based mechanism of its origin. A classical model of the S-shaped
105 population growth is the Verhulst model, but it is completely non mechanistic black-box model,
106 as the internal structure of the system and mechanisms remain hidden.

METHODS

107

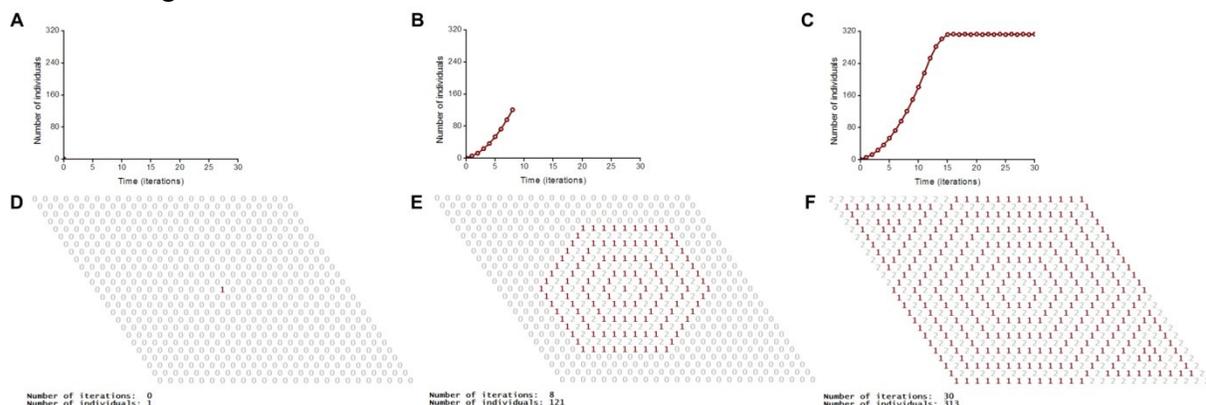
Biological prototype of the model

108

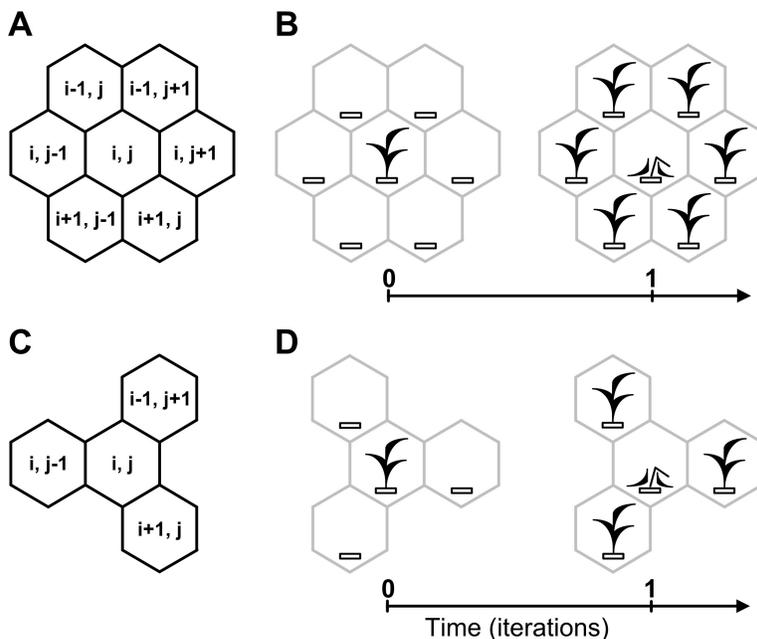
109 A vegetative propagation of rhizomatous lawn grasses is the biological prototype of our model
110 (Fig. 3). Festuca rubra trichophylla (Slender creeping red fescue) is the prototype of aggressive
111 vegetative propagation and Poa pratensis L. and Festuca rubra L. ssp. Rubra are the prototypes of
112 moderate vegetative propagation. One individual corresponds to one tiller. A tiller is a minimal
113 semi-autonomous grass shoot that sprouts from the base. Rhizomes are horizontal creeping
114 underground shoots using which plants vegetatively (asexually) propagate. Unlike a root,
115 rhizomes have buds and scaly leaves. One tiller may have maximum three (Fig. 3D) or six
116 rhizoms (Fig. 3B) in the model. Three rhizoms per tiller correspod to moderate propagation and
117 six rhizoms per tiller correspond to aggressive vegetative propagation. A tiller with roots and
118 leaves develops from a bud on the end of the rhizome. A populated microhabitat goes into the
119 regeneration state after an individual's death. The regeneration state of a site corresponds to the
120 regeneration of microhabitat's resources including recycling of a dead individual (Fig. 4). All
121 individuals are identical. Propagation of offsprings of one individual leads to colonization of the
122 uniform, homogeneous and limited habitat (Fig. 2 and Movies S5-S8).

The cellular automata model

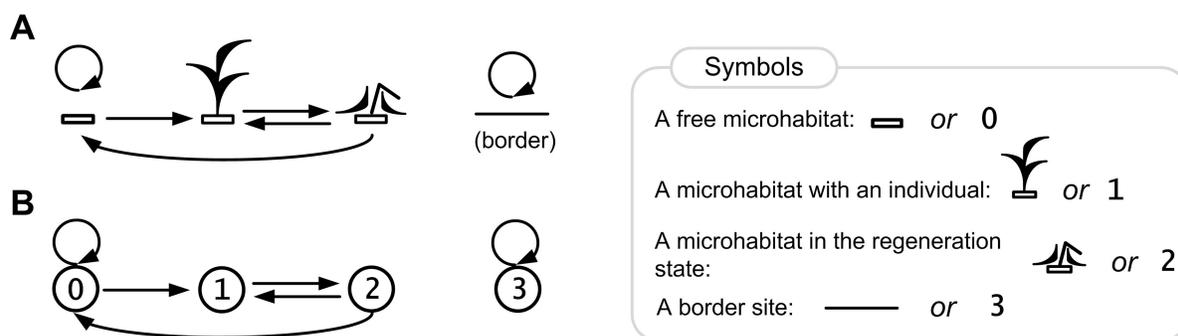
123

124 We use our logical deterministic individual-based cellular automata to model the S-shaped
125 population growth mechanistically. Three patterns of population dynamics of this model are
126 shown in Fig. 2.

127 **Figure 2: S-shaped population growth.** A logical deterministic individual-based cellular
128 automata model of an ecosystem with one species shows both population dynamics and
129 pattern formation. The lattice consists of 25x25 sites. Individuals use the hexagonal
130 neighborhood for propagation. The lattice is closed on the torus to avoid boundary
131 effects. (**A-C**) Population dynamics of the species. S-shaped population growth curve

132   (C). (**D-F**) Spatio-temporal patterns of the model represented in numerical form of
133   program implementation.

134   The presented cellular automata model is defined by the 4-tuple:
135   1. a lattice of sites;
136   2. a set of possible states of a lattice site;
137   3. a neighborhood;
138   4. rules of transitions between the states of a lattice site.
139   The best example of white-box mechanism is a mechanical watch. Our model metaphorically
140   resembles a mechanical watch in transparent case. A neighborhood logically binds dynamics of
141   all cellular automata sites into one holistic complex dynamic system. There are three most known
142   cellular-automamta neighborhoods: von Neumann, Moore and hexagonal. The neighborhood may
143   be of any type. Here we use the hexagonal and tripod neighborhoods which allow to model
144   aggressive and moderate vegetative propagation of rhizomatous lawn grasses (Fig. 3). Different
145   configurations of tripod patterns in Figs 3C and 3D is a result of the fact that the cellular
146   automata neighborhood is implemented successively for each lattice site.

147   **Figure 3: Cellular automata neighborhoods.** A cellular automata neighborhood
148   models a vegetative propagation of plants and defines fecundity and spatial positioning
149   of an individual's offsprings. Coordinates i and j are integer numbers. Positioning of
150   offsprings is explained by how the cellular automata neighborhood is implemented
151   successively for each lattice site. (**A**) Hexagonal neighborhood. (**B**) A model example of
152   vegetative propagation of an individual in the hexagonal neighborhood. Offsprings

153 occupy all nearest lattice sites what corresponds to aggressive propagation. A maximum
154 number of offsprings per one individual (fecundity) equals six. (**C**) Tripod neighborhood.
155 (**D**) A model example of vegetative propagation of an individual in the tripod
156 neighborhood. Offsprings occupy a half of the nearest lattice sites what corresponds to
157 the moderate propagation. A maximum number of offsprings per one individual equals
158 three.

159 A pure mechanistic model of a complex system is a discrete logical model consisting of cause-
160 effects relations and part-whole relations. The causes are sufficient to understand their effects and
161 the parts are sufficient to understand the whole. This mechanistic model is hierarchically
162 subdivided into micro-subsystems, meso-subsystems and a whole macro-system. Interactions
163 between subsystems of a complex system lead to emergence of its new properties. Figs 3 and 4
164 illustrate rules of our basic model. Logical calculations are realized for micro-levels, meso-levels
165 and macro-levels of complex system on each iteration of the cellular automata what may be
166 considered as hyper-logical calculations or automatic hyper-logical inference.

167 **Figure 4: Rules of the ecosystem model with one species.** Directed graph of
168 transitions between the states of a lattice site is represented in pictorial (A) and
169 numerical forms (B). The graph represents a birth-death-regeneration process.

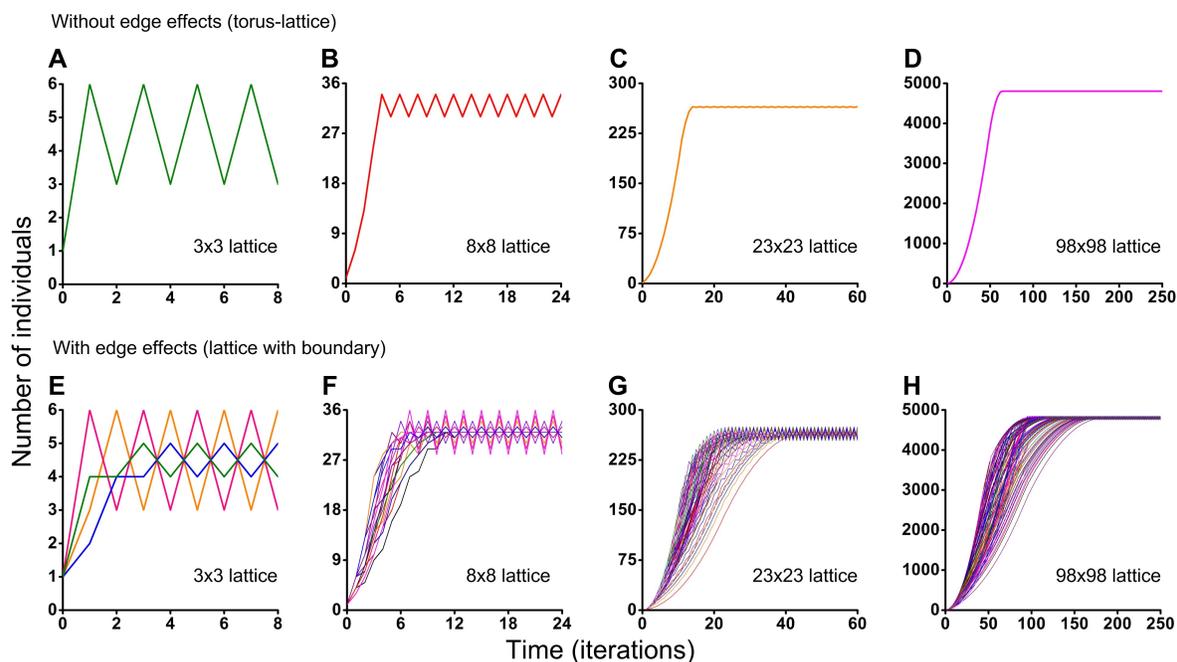
170 Here we show a description of the states of the single species model. Each site may be in one of
171 the four states 0, 1, 2, 3 (Fig. 4), where:
172   0 – a free microhabitat which can be occupied by an individual of the species;
173   1 – a microhabitat is occupied by a living individual of the species;
174   2 – a regeneration state of a microhabitat after death of an individual of the species;
175   3 – a site in this state represents an element of the boundary conditions, i.e. a border.
176 A free microhabitat is the intrinsic part of environmental resources per one individual and it
177 contains all necessary resources and conditions for an individual's life. A microhabitat is modeled
178 by a lattice site.
179 The cause-effects relations are logical rules of transitions between the states of a lattice site (Fig.
180 4B):
181   0→0, a microhabitat remains free if there is no one living individual in its neighborhood;

182 0→1, a microhabitat will be occupied by an individual of the species if there is at least
183 one individual in its neighborhood;
184 1→2, after death of an individual of the species its microhabitat goes into the regeneration
185 state;
186 2→0, after the regeneration state a microhabitat becomes free if there is no one living
187 individual in its neighborhood;
188 2→1, after the regeneration state a microhabitat is occupied by an individual of the
189 species if there is at least one individual in its neighborhood;
190 3→3, a site remains in this state, which defines a border site.

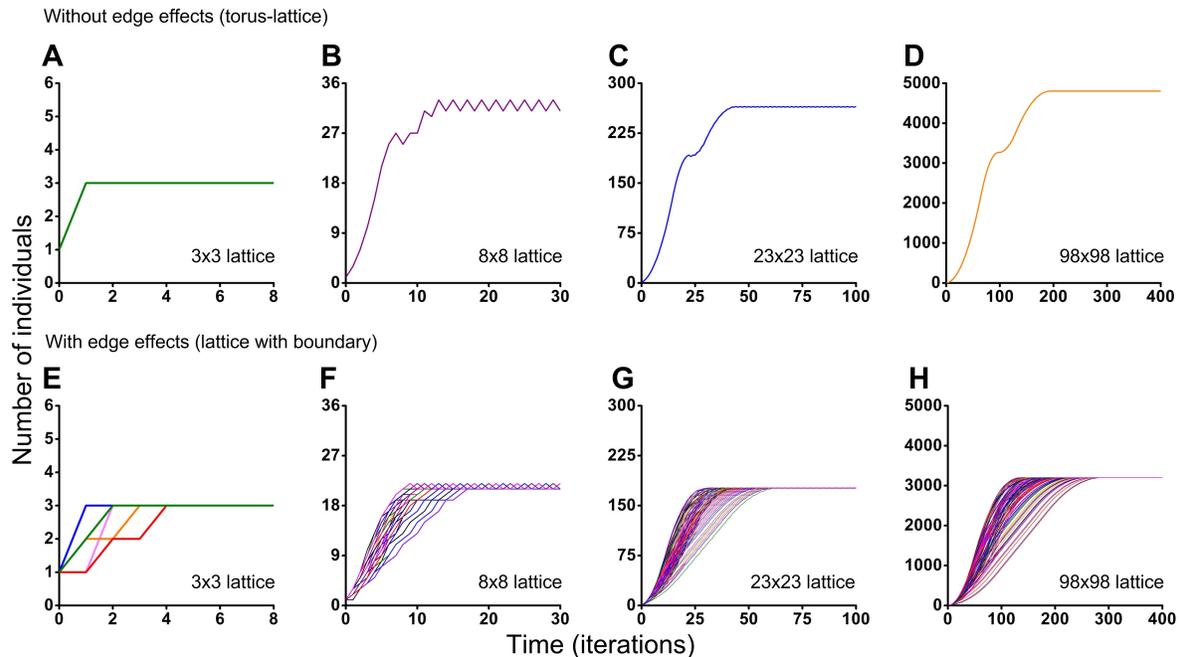
RESULTS AND DISCUSSION

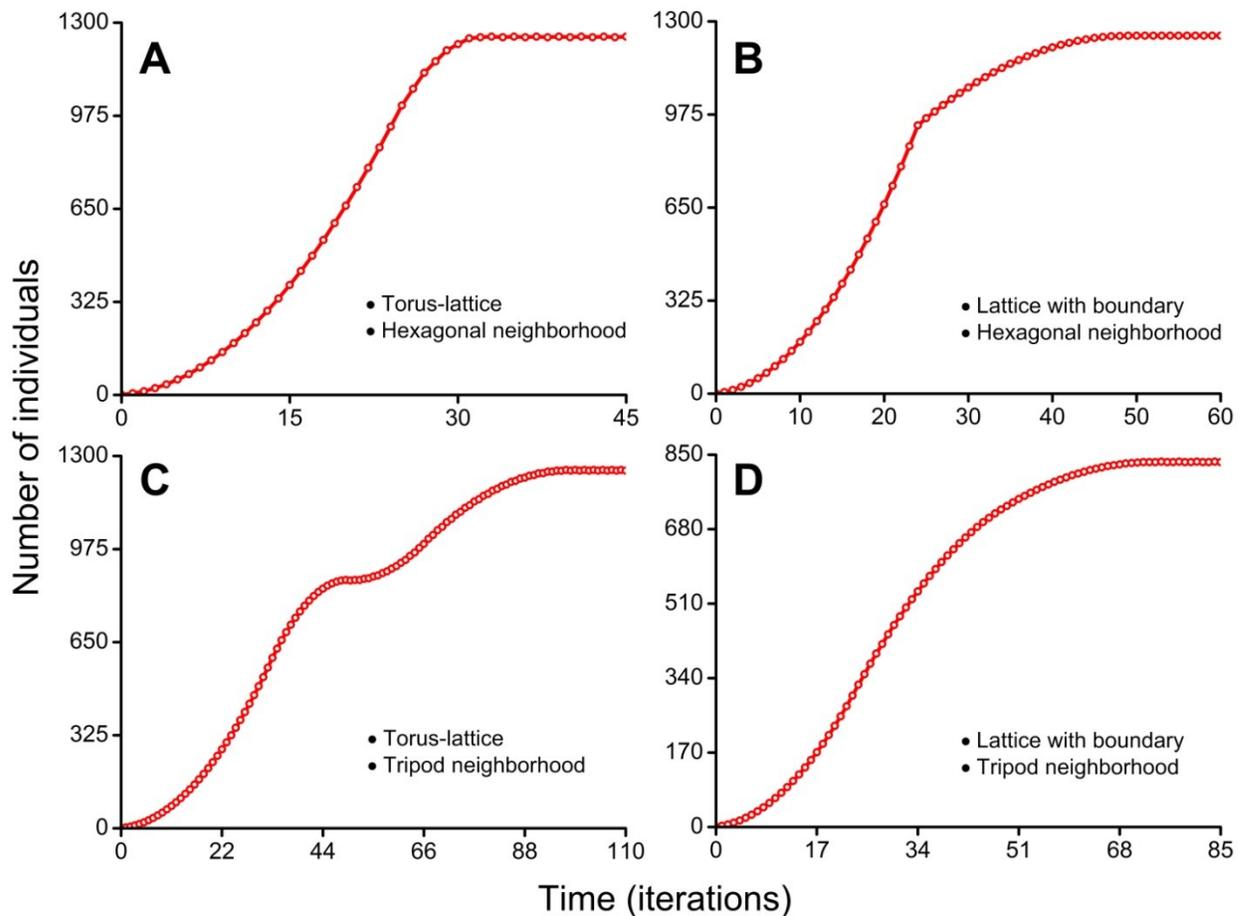
191 **RESULTS AND DISCUSSION**

192 According to Alexander Watt, a plant community may be considered '*as a working mechanism*'
193 which '*maintains and regenerates itself*' (Watt 1947). Our model demonstrates a such
194 mechanism in the most simplified form. From a more general physical point of view we model an
195 active (excitable) media with autowaves (travelling waves, self-sustaining waves) (Kalmykov &
196 Kalmykov 2013; Krinsky 1984; Zaikin & Zhabotinsky 1970). Active medium is a medium that
197 contains distributed resources for maintenance of autowave propagation. An autowave is a self-
198 organizing and self-sustaining dissipative structure. An active medium may be capable to
199 regenerate its properties after local dissipation of resources. In our model, propagation of
200 individuals occurs in the form of population waves. We use the axiomatic formalism of Wiener
201 and Rosenblueth for modeling of excitation propagation in active media (Wiener & Rosenblueth
202 1946). In accordance with this formalism rest, excitation and refractoriness are the three
203 successive states. In our formalism the rest state corresponds to the free state of a microhabitat,
204 the excitation state corresponds to the life activity of an individual in a microhabitat and the
205 refractory state corresponds to the regeneration state of a microhabitat. All states have identical
206 duration. If the refractory period will be much longer than the active period, then such a model
207 may be interpreted, for example, as propagation of the single wave of dry grass fire. Time
208 duration of the basic states can be easily varied using additional states of the lattice sites.
209 Different initial conditions may lead to formation of different spatio-temporal patterns and as a
210 result they may lead to different dynamics of the system. Using the Monte Carlo method, we
211 have investigated the influence of different initial conditions on population dynamics of one
212 species. We have investigated two different boundary conditions, two different cellular automata
213 neighborhoods and four different lattice sizes (Figs 5 and 6). Different cellular automata
214 neighborhoods allowed us to investigate aggressive and moderate variants of vegetative
215 propagation of rhizomatous lawn grasses. Aggressive propagation was modeled by the hexagonal
216 neighborhood (Fig. 3A), where an individual's offsprings may occupy all nearest microhabitats
217 (Fig. 3B). Moderate propagation was modeled using the tripod neighborhood (Fig. 3C), where an
218 individual's offsprings may occupy only a half of the nearest microhabitats (Fig. 3D). Figure 5
219 shows the results obtained in the study of aggressive propagation and Figure 6 shows the results
220 obtained in the study of moderate propagation. In Figs 5B-D and 6E-H we show the S-shaped

221   population growth and in Fig. 6B-D we show the double S-shaped population growth. Sizes of
222   the lattice which define available space for colonization consisted of 3x3, 8x8, 23x23 and 98x98
223   sites. We investigated the boundary conditions of two types when the lattice was closed on the
224   torus by periodic conditions (Fig 5A-D and Fig 6A-D) and when the lattice has a boundary (Fig
225   5E-H and Fig 6E-H). There were no changes of population dynamics in result of the different
226   initial positioning of an individual on the lattice in cases with periodic boundary conditions (Fig
227   5A-D and Fig 6A-D). In cases when a lattice has a boundary, different initial positioning of an
228   individual lead to differences in population dynamics (Fig 5E-H and Fig 6E-H). Moreover,
229   increasing of the lattice may lead to more complex dynamics (Figs 5E-H, 6E-H).
230   Periodic fluctuations in numbers of individuals are observed at the plateau phase in most of the
231   experiments. With increasing of the lattice size, these periodic fluctuations in population size
232   become less visible. The periodic fluctuations on the plateau phase are absent when the lattice
233   consists of 3x3 sites in the case of the tripod neighborhood (Fig. 6A, 6E). The similar plateau
234   phases without fluctuations were found at the 3Nx3N sizes of the lattice (6x6, 9x9, 12x12, 15x15,
235   18x18, 27x27 lattices were tested), with and without edge effects and when the neighborhood
236   was tripod.

237   **Figure 5: Results of the Monte Carlo simulations with hexagonal neighborhood.**
238   Investigation of the influence of boundary conditions, initial positioning of an individual
239   and lattice sizes on single-species population dynamics. (**A-D**) The lattice is closed on
240   the torus to avoid boundary effects. (**E-H**) The lattice has a boundary. Every Monte Carlo
241   simulation consisted of 100 repeated experiments with different initial positioning of an
242   individual on the lattice.

243   As examples of the Monte Carlo simulation we show four Movies S1-S4. Each Monte Carlo
244   simulation consists of five repeated experiments with different initial positioning of an individual

245   on the lattice. The lattices are uniform, homogeneous and limited in all experiments. They are
246   consisted of 23x23 sites available for occupation by individuals. In Movie S1 the lattice is closed
247   on the torus and the neighborhood is hexagonal. In Movie S2 the lattice has a boundary and the
248   neighborhood is hexagonal. In Movie S3 the lattice is closed on the torus and the neighborhood is
249   tripod. In Movie S4 the lattice has a boundary and the neighborhood is tripod.

250   **Figure 6: Results of the Monte Carlo simulations with tripod neighborhood.**
251   Investigation of the influence of boundary conditions, initial positioning of an individual
252   and lattice sizes on single-species population dynamics. (**A-D**) The lattice is closed on
253   the torus to avoid boundary effects. (**E-H**) The lattice has a boundary. Every Monte Carlo
254   simulation consisted of 100 repeated experiments with different initial positioning of an
255   individual on the lattice.

256   In more detail different spatio-temporal mechanisms we present the double S-shaped population
257   growth curve (Fig. 7, Movie S7) and three types of the S-shaped population growth curves. (Fig.
258   7, Movies S5,S6,S8).

259   **Figure 7: Population growth curves.** The lattice size which is available for occupation
260   consisted of 50x50 sites in all four cases. (**A**) S-shaped curve with short phase of
261   decelerating growth. Cellular automata neighborhood is hexagonal and the lattice is
262   closed on the torus (Movie S5). (**B**) S-shaped curve with sharp transition to long phase
263   of decelerating growth. Cellular automata neighborhood is hexagonal and the lattice has
264   a boundary (Movie S6). (**C**) Double S-shaped population growth curve. Cellular
265   automata neighborhood is tripod and the lattice is closed on the torus (Movie S7). (**D**) S-
266   shaped curve with very long phase of decelerating growth. Cellular automata
267   neighborhood is tripod and the lattice has a boundary (Movie S8).

268   Figure 7A shows the S-shaped population growth curve with short phase of decelerating growth.
269   This curve reaches a plateau earlier than on population curves in Figures 7B-D. The plateau is
270   reached on the 32nd iteration (Movie S5). The higher rate of population growth is explained by
271   aggressive propagation and by the lack of edge effects.
272   Figure 7B shows the S-shaped population growth curve with sharp transition to long phase of
273   decelerating growth. This curve has a sharp slowdown of population growth before beginning of
274   phase of decelerating growth. It occurs on the 25th iteration, when population waves of
275   aggressively propagating species reach the habitat boundaries (Movie S6). In contrast to the
276   curve in Figure 7A, this population curve reaches the plateau on the 49th iteration. Reduced
277   population growth rate of aggressively propagating species is explained by the presence of edge
278   effects.

279   In Figure 7C the population growth curve has a double S-shaped form. The double S-shaped
280   population growth is a result of temporary slowdown of growth, which occurs at the stage when
281   colonization of the free field is replaced by interpenetration of colliding population waves into
282   already occupied areas. Starting from the 34th iteration, the stage of gradually compaction of
283   populated areas begins (Movie S7). This compaction arises from the fact that after rounding of
284   the torus population waves occupy the remaining free sites in the partially populated part of
285   habitat as result of a 'phase shift' of the colliding waves. The free vacancies in population waves
286   remain in result of moderate propagation of individuals. The moderate propagation is modeled by
287   the tripod neighborhood. Speed of the sealing colonization increases slowly due to the form of
288   the population waves which invade into already occupied areas by the expanding wedge. At the
289   same time contribution into population growth from colonization of the areas which consists only
290   of free microhabitats decreases. The areas which consist only of free microhabitats disappear on
291   the 49th iteration. The population growth rate temporarily slows down what forms the first
292   plateau of the curve. This plateau phase lasts during 5 iterations. The accelerating of additional
293   compactization of population waves leads to the new population growth starting from the 53rd
294   iteration. The population curve reaches the second plateau on the 98th iteration.
295   Figure 7D shows the S-shaped population growth curve with very long phase of decelerating
296   growth. This curve reaches a plateau on the 72nd iteration (Movie S8). Reduced population
297   growth rate and reduced maximum number of individuals in the habitat (834 individuals) are a
298   result of the boundary conditions and with the moderate fecundity of individuals (because of
299   tripod neighborhood).

300   We have investigated population growth limited by different factors, e.g. finite size of the habitat
301   (limited resources), its forms, intraspecific competition, lifetime of individuals, regeneration time
302   of microhabitats, fecundity of individuals (Figs 2, 5-7 and Movies S1-S8). Here we show the
303   model of J-shaped population growth and investigate two cases of geometric population growth.
304   Unlike of the S-shaped population model, the J-shaped population model describes a situation in
305   which population growth is not limited in resources, for environmental reasons or by existence of
306   competitors, predators, herbivores and diseases. J-shaped population model describes a full
307   reproductive potential which lead to geometrical population growth (Fig. 8). In other respects this
308   model corresponds with our model of S-shaped population growth. It also takes into account
309   natural decline of individuals. Individual's lifetime equals one iteration.

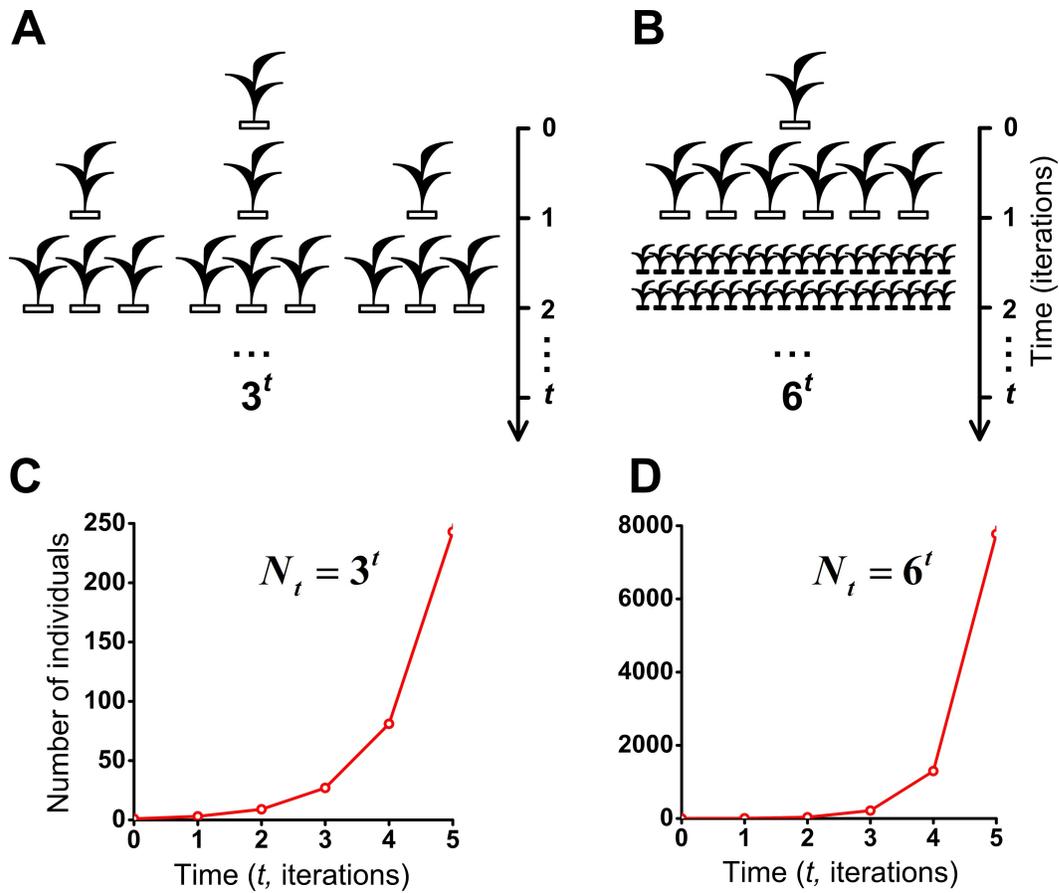



Figure 8: J-shaped population growth model. Propagation of individuals occurs in the absence of intraspecific competition and any restrictions on the resources. A species colonizes an infinite ecosystem under ideal conditions. (**A**) The number of offsprings per individual equals three. (**B**) The number of offsprings per individual equals six. (**C**) Geometric population growth in the first case (A). (**D**) Geometric population growth in the second case (B).

To assess the effect of intraspecific competition and regeneration of microhabitats on population growth we compared our model of the S-shaped growth (Fig. 7A and Movie S5) with the J-shaped model of population growth in the presence of unlimited resources and without intraspecific competition (Fig. 8B, D). Comparative dynamics of these models is shown in Table 1. Comparison of these two examples shows that intraspecific competition is a powerful factor which limits population growth. We also compared our double S-shaped population growth model (Fig. 7C and Movie S7) with the J-shaped population growth model (Fig. 8A, C). Comparative dynamics of these models is shown in Table 2. Thus, we have compared our models of S-shaped and double S-shaped population growth with the J-shaped population growth.

325 **Table 1: Comparative population dynamics in the models with the S-shaped and**
326 **the J-shaped population growth.**

Time (Number of iteration and generation)	0	1	2	3	4	5
Number of individuals in the S-shaped population growth model (Fig. 7A and Movie S5). Intraspecific competition exists. Fecundity equals 6 individuals.	1	6	13	24	37	54
Number of individuals in the J-shaped population growth model (Fig. 8B,D). Intraspecific competition is absent. Geometric population growth. Fecundity equals 6.	1	6	36	216	1296	7776

327 **Table 2: Comparative population dynamics in the models with the double S-**
328 **shaped and the J-shaped population growth.**

Time (Number of iteration and generation)	0	1	2	3	4	5
Number of individuals in the S-shaped population growth model (Fig. 7C and Movie S7). Intraspecific competition exists. Fecundity equals 3.	1	3	6	10	15	21
Number of individuals in the J-shaped population growth model (Fig. 8A,C). Intraspecific competition is absent. Geometric population growth. Fecundity equals 3.	1	3	9	27	81	243

329 The basic ecological model, which presented in this paper, can easily be expanded by the
330 introduction of additional states, different neighborhoods, nested and adjoint lattices (Kalmykov
331 & Kalmykov 2012). Such extension has allowed us to create pure mechanistic models of
332 interspecific competition between two, three and four species that are complete competitors, and
333 then to verify and reformulate the competitive exlusion principle (Kalmykov & Kalmykov 2013)
334 in order to solve the biodiversity mystery (Sommer 1999).

335 **CONCLUSIONS**

336 We have presented and investigated a mechanistic model of single species population dynamics.
337 This model is based on pure logical deterministic individual-based cellular automata. It has a
338 physical and ecological ontology of part-whole and cause-effects relations. A physical ontology is

339   the ontology of the active medium and ecological ontology represents an ecosytem with the plant
340   community. This is a white-box model of single-species population dynamics. The presented
341   model gives a strong mechanistic insight of the S-shaped and double S-shaped population
342   growth. This model provides mechanistic fundamentals for population dynamics. It is useful as a
343   starting point for pure mechanistic modeling of population and ecosytem dynamics of more
344   complex situations like interspecific competition. Our deterministic logical cellular automata
345   model work as a system of artificial intelligence. It hyper-logically provides automatic deductive
346   inference. Instead of single logical steps, built up to a linear logical sequence, the program may
347   iteratively perform parallel logical operations in all sites of the cellular automata lattice. We
348   consider that the main difficulty of this white-box modeling is to create an adequate axiomatic
349   system based on an intrinsic physical ontology of the complex system under study. The main
350   feature of the approach is the use of cellular automata as a way of linking semantics (ontology)
351   and logic of the subject area. Here we have created and investigated a logical white-box model of
352   an ecosystem with one species, which combines reductionist and holistic approaches to the
353   modeling of complex systems. Integration of reductionist and holistic approaches is provided by
354   the simultaneous modeling of both part-whole and cause-effect relations in complex system. We
355   consider the white-box modeling by logical deterministic cellular automata as a perspective way
356   for investigation not only of population dynamics but also of all complex systems.

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359   **Supplemental Information** Movies S1-S8 can be found online.

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