A white-box model of S-shaped and double S-shaped single-species population growth

Lev V. Kalmykov, Vyacheslav L. Kalmykov

Background. A mechanistic modeling of complex systems is one of the main scientific problems today. We consider that this problem may be solved by white-box modeling with using logical deterministic cellular automata. Mathematical models of complex systems are divided into three types: black-box (phenomenological), white-box (mechanistic, based on the first principles) and grey-box (mixtures of phenomenological and mechanistic models). Most basic ecological models are of black-box type, including Malthusian, Verhulst, Lotka-Volterra models. The problem is that the using these black-box models may give us only phenomenological mechanisms, but individual-based (mechanistic) mechanisms of population dynamics remain hidden. Our main goal here is to show possibilities of the white-box modeling in investigating mechanisms of S-shaped and double S-shaped population growth of vegetatively propagated plants. **Methods.** Using purely logical deterministic individual-based cellular automata we create a white-box model of vegetatively propagated plants. From a general physical standpoint the vegetative propagation of plants is an analogue of excitation propagation in excitable media. 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 sizes of the habitat, two types of fecundity and two types of boundary conditions. **Results.** We have created and investigated a basic mechanistic model of one-species population dynamics. This model demonstrates individual-based mechanisms of the S-shaped and double S-shaped population growth. We have investigated mechanisms of the single-species population growth limited by different factors, in particular by resources, habitat size, intraspecific competition, lifetime of individuals, regeneration time and fecundity of individuals. Besides that we have compared the S-shaped and J-shaped population growth. **Conclusion.** The model demonstrates deterministic individual-based mechanisms of the S-shaped and double S-shaped population growth of vegetatively propagated rhizomatous lawn grasses. An additional important result is a novel demonstration of the white-box modeling of the ecosystem using logical deterministic individual-based cellular automata. We consider this white-box modeling approach as a perspective method of artificial intelligence which works

as automatic hyper-logical inference from the first principles of the studied subject. This approach may provide direct mechanistic insights into any complex systems.

A white-box model of S-shaped and double S-shaped single-species population growth

Lev V. Kalmykov[1], Vyacheslav L. Kalmykov[2,3]

[1]Institute of Theoretical and Experimental Biophysics, Russian Academy of Sciences, 142290 Pushchino, Moscow Region, Russian Federation

[2]Institute of Cell Biophysics, Russian Academy of Sciences, 142290 Pushchino, Moscow Region, Russian Federation

[3]Pushchino State Institute of Natural Sciences, 142290 Pushchino, Moscow Region, Russian Federation

Corresponding author Vyacheslav L. Kalmykov, vyacheslav.l.kalmykov@gmail.com

ABSTRACT

Background. A mechanistic modeling of complex systems is one of the main scientific problems today. We consider that this problem may be solved by white-box modeling with using logical deterministic cellular automata. Mathematical models of complex systems are divided into three types: black-box (phenomenological), white-box (mechanistic, based on the first principles) and grey-box (mixtures of phenomenological and mechanistic models). Most basic ecological models are of black-box type, including Malthusian, Verhulst, Lotka-Volterra models. The problem is that the using these black-box models may give us only phenomenological mechanisms, but individual-based (mechanistic) mechanisms of population dynamics remain hidden. Our main goal here is to show possibilities of the white-box modeling in investigating mechanisms of S-shaped and double S-shaped population growth of vegetatively propagated plants.

Methods. Using purely logical deterministic individual-based cellular automata we create a white-box model of vegetatively propagated plants. From a general physical standpoint the vegetative propagation of plants is an analogue of excitation propagation in excitable media. 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 sizes of the habitat, two types of fecundity and two types of boundary conditions.

Results. We have created and investigated a basic mechanistic model of one-species population dynamics. This model demonstrates *individual-based mechanisms* of the S-shaped and double S-shaped population growth. We have investigated mechanisms of the single-species population growth limited by different factors, in particular by resources, habitat size, intraspecific competition, lifetime of individuals, regeneration time and fecundity of individuals. Besides that we have compared the S-shaped and J-shaped population growth.

Conclusion. The model demonstrates deterministic individual-based mechanisms of the S-shaped and double S-shaped population growth of vegetatively propagated rhizomatous lawn grasses. An additional important result is a novel demonstration of the white-box modeling of the ecosystem using logical deterministic individual-based cellular automata. We consider this white-box modeling approach as a perspective method of artificial intelligence which works as automatic

38 hyper-logical inference from the first principles of the studied subject. This approach may
39 provide direct mechanistic insights into any complex systems.

40 **Keywords:** population dynamics, complex systems, cellular automata, individual-based
41 modeling, population growth curves, population waves, artificial intelligence

INTRODUCTION

Background

44 A mechanistic approach corresponds to the classical ideal of science. Existing mathematical
45 approaches to complex systems modeling are rather phenomenological than mechanistic.
46 Ecologists investigate population dynamics phenomenologically, rather than mechanistically
47 (Tilman 1987). Nonmechanicalness (phenomenologicalness) is still a characteristic for
48 mathematical modeling of complex systems. Most mathematical models in ecology, from simple
49 equations of population growth to complex descriptions of ecosystem dynamics, are not
50 individual-based, i.e. they do not model individuals and their local interactions (Huston et al.
51 1988). The purpose of this study is a mechanistic investigation of the S-shaped and double S-
52 shaped population growth. Individual-based mechanisms of the S-shaped and double S-shaped
53 population growth of vegetatively propagated plants should be completely discrete, logical and
54 consisting of cause-effect and of part-whole relations between micro-subsystems, meso-
55 subsystems and a whole macro-system.

On the types of mathematical models of complex systems

57 How to create an individual-based mechanistic model of population growth? First, we need to
58 know how to mechanistically model a complex dynamic system. A complex dynamic system may
59 be considered as consisting of interacting subsystems. Interactions between subsystems lead to
60 the emergence of new properties, e.g. of a new pattern formation. Therefore we should define
61 these subsystems and logically describe their interactions in order to create and investigate a
62 mechanistic model. If we want to understand how a complex dynamic system works, we must
63 understand cause-effect relations and part-whole relations in this system. The causes should be
64 sufficient to understand their effects and the parts should be sufficient to understand the whole.
65 There are three types of possible models for complex dynamic systems: black-box, grey-box and
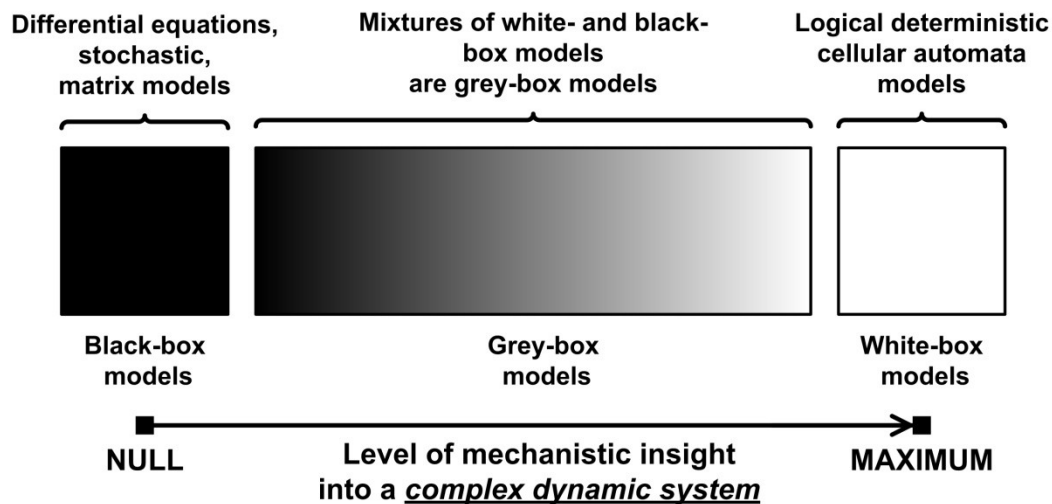66 white-box models (Fig. 1).

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

70   Black-box models are completely nonmechanistic. They are phenomenological and ignore a
71   composition and internal structure of a complex system. We cannot investigate interactions of
72   subsystems of such a non-transparent model. A of complex dynamic systems has 'transparent
73   walls' and directly shows underlying mechanisms. All events at micro-, meso- and macro-levels
74   of a dynamic system are directly visible at all stages of its white-box model. Unfortunately, in
75   most cases mathematical modelers prefer to use the heavy black-box mathematical methods,
76   which cannot produce mechanistic models of complex dynamic systems in principle. Grey-box
77   models are intermediate and combine black-box and white-box approaches. As a rule, this
78   approach is used in 'overloaded' form, what makes it less transparent. Basic ecological models
79   are of black-box type, e.g. Malthusian, Verhulst, Lotka-Volterra models. These models are not
80   individual-based and cannot show features of local interactions of individuals of competing
81   species. That is why they principally cannot provide a mechanistic insight into dynamics of
82   ecosystems. Earlier we demonstrated, that the logical deterministic cellular automata approach
83   allows to create the white-box models of ecosystems with interspecific competition between two,
84   three and four grass species (Kalmykov & Kalmykov 2013). A similar cellular automata model of
85   interspecific competition was created by Silvertown and colleagues (Silvertown et al. 1992).
86   Their model simulates competitive interactions of five grass species, based on experimentally
87   determined rates of invasion. This is a grey-box model as it is based on complex stochastic rules
88   of interspecific interactions. Another similar cellular automata model of single plant species was
89   proposed by Komarov and colleagues, where they represented a link between the concept of
90   discrete description of the ontogenesis of plants and the cellular automata (Komarov et al. 2003).
91   The both two models (Komarov et al. 2003; Silvertown et al. 1992) do not take into account
92   regeneration processes of an ecosystem.

93   Creation of a white-box model of complex system is associated with the problem of the necessity
94   of an a priori basic knowledge of the modeling subject. The deterministic logical cellular
95   automata are necessary but not sufficient condition of a white-box model. The second necessary
96   prerequisite of a white-box model is the presence of the physical ontology of the object under
97   study. The white-box modeling represents the automatic hyper-logical inference from the first
98   principles because it is completely based on the deterministic logic and axiomatic theory of the
99   subject. The purpose of the white-box modeling is to derive from the basic axioms a more
100   detailed, more concrete mechanistic knowledge about the dynamics of the object under study. We
101   see no other way to obtain a specific and, at the same time, holistic mechanistic understanding of
102   complex systems, apart from the white-box modeling. For providing a strong relevance of our
103   model to the studied problem, we have specified the models' rules (axioms) strictly in accordance
104   with the subject under study. Each logical rule of the model has a correct ecological and physical
105   interpretation. From an ecological point of view we model a vegetative propagation of
106   rhizomatous lawn grasses. From a physical point of view we model propagating of excitation
107   (autowaves, travelling waves, self-sustaining waves) in an excitable (active) medium. The
108   presence of such physical interpretation makes our specific ecological model more general and
109   more natural. The necessity to formulate an intrinsic axiomatic system of the subject before
110   creating its white-box model distinguishes the cellular automata models of white-box type from
111   cellular automata models based on arbitrary logical rules. If cellular automata rules have not been
112   formulated from the first principles of the subject, then such a model may have a weak relevance
113   to the real problem.

On the white-box modeling of population dynamics

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

121   Stephen Hubbell in his Unified Neutral Theory of Biodiversity (UNTB) in fact refuses a
122   mechanistic understanding of interspecific competition: '*We no longer need better theories of*
123   *species coexistence; we need better theories for species presence-absence, relative abundance*
124   *and persistence times in communities that can be confronted with real data. In short, it is long*
125   *past time for us to get over our myopic preoccupation with coexistence'* (Hubbell 2001).
126   However, he admits that '*the real world is not neutral'* (Rosindell et al. 2012). Since the basic
127   postulate of the UNTB about ecological neutrality of the similar species in the ecosystem is
128   wrong, this theory cannot be true. In addition, direct local interactions of individuals are absent in
129   the neutral models in principle. That is why neutral models cannot provide a mechanistic insight
130   into biodiversity. The UNTB models are of black-box and dark grey-box types only – Fig. 1. We
131   agree with James Clark, that the dramatic shift in ecological research to focus on neutrality
132   distracts environmentalists from the study of real biodiversity mechanisms and threats (Clark
133   2009). Within the last decade, the neutral theory has become a dominant part of biodiversity

134   science, emerging as one of the concepts most often tested with field data and evaluated with
135   models (Clark 2009). Neutralists are focused on considering unclear points of the neutral theory –
136   the ecological drift, the link between pattern and process, relations of simplicity and complexity
137   in modeling, the role of stochasticity and others, but not the real biodiversity problems
138   themselves (Rosindell et al. 2012). Attempts to understand neutrality instead of biodiversity
139   understanding look like attempts to explain the obscure by the more obscure. Nonmechanistic
140   ecological models make it difficult to answer basic questions, e.g. Why are there so many closely
141   allied species? (Anonymous 1944) An example of the difficult ecological discussion is the
142   debates 'Ecological neutral theory: useful model or statement of ignorance?' on the forum Cell
143   Press Discussions (Craze 2012).Understanding of mechanisms of interspecific coexistence is a
144   global research priority. These mechanisms can allow us to efficiently operate in the field of
145   biodiversity conservation. Obviously, such knowledge must be based on mechanistic models of
146   species coexistence. Unfortunately, ecological modelers prefer to use the heaviest black-box
147   mathematical methods, which cannot produce mechanistic models of complex dynamic systems
148   in principle, and not use simple and long-known purely logical deterministic cellular automata,
149   which can produce white-box models and directly obtain clear mechanistic insights into
150   dynamics of complex systems.

METHODS

151

Biological prototype of the model

152

153   A vegetative propagation of rhizomatous lawn grasses is the biological prototype of our model
154   (Fig. 3). *Festuca rubra trichophylla* (*Slender creeping red fescue*) is the prototype of aggressive
155   vegetative propagation and *Poa pratensis* L. and *Festuca rubra* L. *ssp. Rubra* are the prototypes
156   of moderate vegetative propagation. One individual corresponds to one tiller. A tiller is a minimal
157   semi-autonomous grass shoot that sprouts from the base. Rhizomes are horizontal creeping
158   underground shoots using which plants vegetatively (asexually) propagate. Unlike a root,
159   rhizomes have buds and scaly leaves. One tiller may have maximum three (Fig. 3D) or six
160   rhizoms (Fig. 3B) in the model. Three rhizoms per tiller correspod to moderate propagation (only
161   a half of the nearest microhabitats) and six rhizoms per tiller correspond to aggressive vegetative
162   propagation. A tiller with roots and leaves develops from a bud on the end of the rhizome. A
163   populated microhabitat goes into the regeneration state after an individual's death. The
164   regeneration state of a site corresponds to the regeneration of microhabitat's resources including
165   recycling of a dead individual (Fig. 4). All individuals are identical. Propagation of offsprings of
166   one individual leads to colonization of the uniform, homogeneous and limited habitat (Fig. 2 and
167   Movies S5-S8).

The cellular automata model

168

169   We have used logical deterministic individual-based cellular automata to model the S-shaped
170   population growth mechanistically (Fig. 2). This model demonstrates the underlined individual-
171   based mechanisms. A classical model of the S-shaped population growth is the Verhulst model,
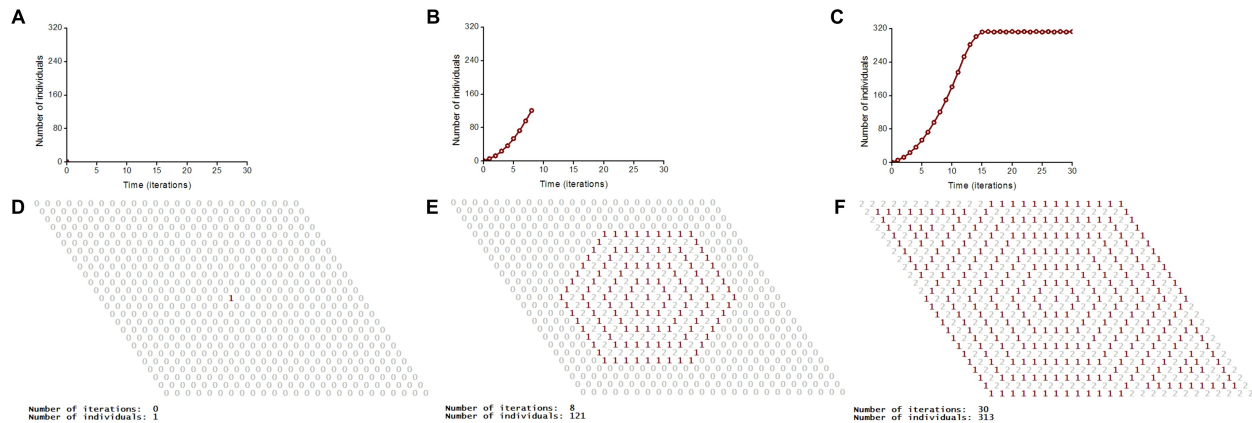172   which is of completely non mechanistic black-box nature.

173 **Figure 2: S-shaped population growth.** A logical deterministic individual-based cellular
174 automata model of an ecosystem with one species shows both population dynamics and
175 pattern formation. The lattice consists of 25x25 sites. Individuals use the hexagonal
176 neighborhood for their vegetative propagation. The lattice is closed on the torus to avoid
177 boundary effects. (**A-C**) Population dynamics of the species. S-shaped population
178 growth curve (**C**). (**D-F**) Spatio-temporal patterns of the model are represented in
179 numerical form of program implementation.

180 The presented cellular automata model is defined by the 4-tuple:
181   1. a cellular automata lattice, uniting a collection of sites;
182   2. a finite set of possible states for each lattice site;
183   3. a cellular automata neighborhood which consists of a site and its intrinsically defined
184   neighbors;
185   4. a function of transitions between the states of a lattice site.
186 The best example of a white-box mechanism is a mechanical watch. Our model metaphorically
187 resembles a mechanical watch in transparent case. A neighborhood logically binds dynamics of
188 all cellular automata sites into one holistic complex dynamic system. There are three most known
189 cellular-automata neighborhoods: von Neumann, Moore and hexagonal. The neighborhood may
190 be of any type. Here we use the hexagonal and tripod neighborhoods which allow to model
191 aggressive and moderate vegetative propagation of rhizomatous lawn grasses (Fig. 3). Different
192 configurations of tripod patterns in Figs 3C and 3D is a result of the fact that the cellular
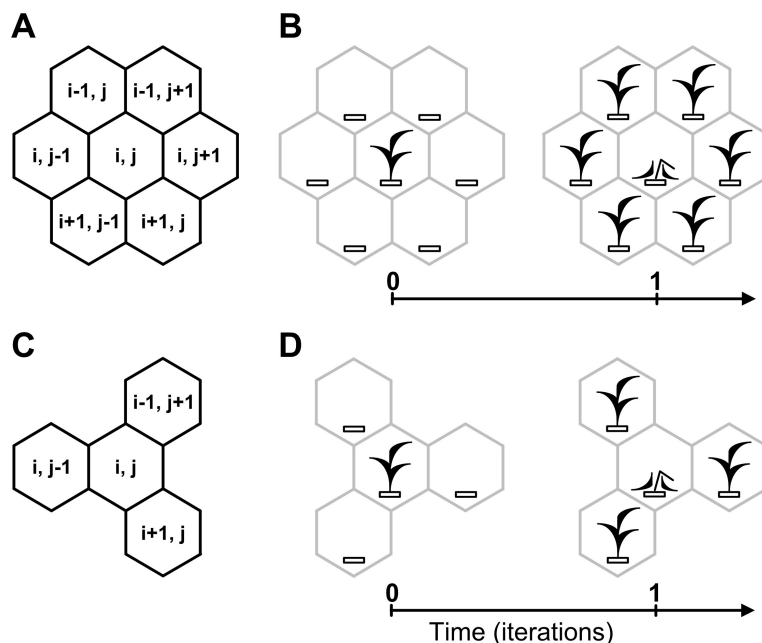193 automata neighborhood is implemented successively for each lattice site.

Figure 3: Cellular automata neighborhoods. A cellular automata neighborhood models a vegetative propagation of plants and defines fecundity and spatial positioning of an individual's offsprings. Positioning of offsprings is explained by how the cellular automata neighborhood is implemented successively for each lattice site. A central site of the neighborhood is defined by the array element with index (i, j), where i and j are integer numbers. Neighboring sites of the central site are defined by the array elements with indexes. (**A**) Hexagonal neighborhood. (**B**) A model example of vegetative propagation of an individual in the hexagonal neighborhood. Offsprings occupy all nearest lattice sites what corresponds to aggressive propagation. A maximum number of offsprings per one individual (fecundity) equals six. (**C**) Tripod neighborhood. (**D**) A model example of vegetative propagation of an individual in the tripod neighborhood. Offsprings occupy a half of the nearest lattice sites what corresponds to the moderate propagation. A maximum number of offsprings per one individual equals three.

Integration of reductionist and holistic approaches is one of the challenges for mathematical modeling. Our white-box model of single-species population dynamics opens up new possibilities to solve this challenge. This mechanistic model is hierarchically subdivided into micro-subsystems, meso-subsystems and the whole macro-system. A micro-level is modeled by lattice sites (cellular automata cells). A meso-level of local interactions of micro-objects is modeled by the cellular automata neighborhood. A macro-level is modeled by the entire cellular automata lattice. This is a 'multy-level' modelling as parallel logical operations performed on micro-level, meso-level and macro-level of the model. A unique feature of the cellular-automata is the possibility to model part-whole relationships mechanistically. The relationships of the parts and the whole are modelled using the transition function (combination of the neigbourhood and rules of transition) between states of a lattice site. Parts are the lattice sites and the whole (ecosystem) is the lattice. On each iteration of evolution of the modeled macrosystem the states of its microsystems are changing simultaneously on the basis of logical ruless taking into account states of the neighbouring microsystems (neigbourhood's sites). This allows to model how interactions of microsystems (parts) produce evolution of the macro-system (whole) which leads

222   to emergence of its new properties (the ecosystem patterns). The white-box cellular automata
223   model shows interactions of parts within the whole, i.e. 'part-whole' relations in the modeled
224   complex system.
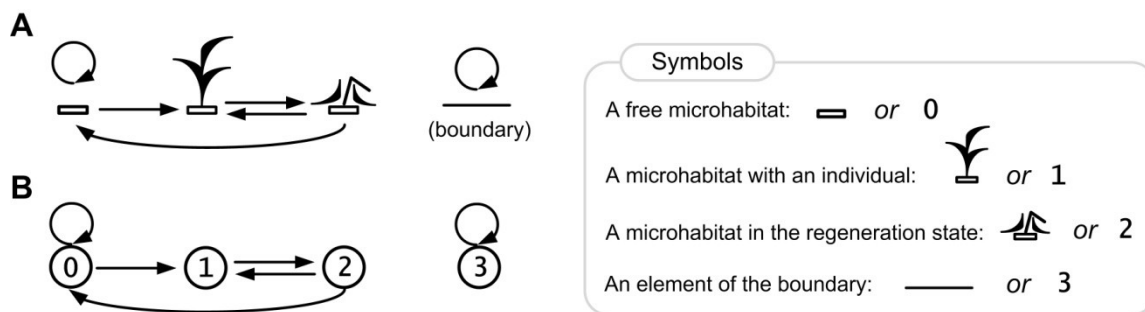225   Figures 3 and 4 illustrate rules of our model.

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

229   Here we show a description of the states of a lattice site (microecosystem) in the single species
230   population growth model. Each site may be in one of the four states 0, 1, 2, 3 (Fig. 4), where:
231   0 – a free microhabitat which can be occupied by an individual of the species;
232   1 – a microhabitat is occupied by a living individual of the species;
233   2 – a regeneration state of a microhabitat after death of an individual of the species;
234   3 – a site in this state represents an element of the boundary that cannot be occupied by an
235   individual.
236   A free microhabitat is the intrinsic part of environmental resources per one individual and it
237   contains all necessary resources for an individual's life. A microhabitat is modeled by a lattice
238   site.
239   The cause-effect relations are logical rules of transitions between the states of a lattice site (Fig.
240   4B):
241   0→0, a microhabitat remains free if there is no one living individual in its neighborhood;
242   0→1, a microhabitat will be occupied by an individual of the species if there is at least
243   one individual in its neighborhood;
244   1→2, after death of an individual of the species its microhabitat goes into the regeneration
245   state;
246   2→0, after the regeneration state a microhabitat will be free if there is no one living
247   individual in its neighborhood;
248   2→1, after the regeneration state a microhabitat will be occupied by an individual of the
249   species if there is at least one individual in its neighborhood;
250   3→3, a site remains in this state, which defines a boundary site.

251   These logical statements are realized for all micro-levels (sites) with their meso-levels
252   (neighborhoods) and thus for the whole macro-level (lattice) of the complex system on each time

253   iteration. We consider implementation of this algorithm as hyper-logical operations or automatic
254   hyper-logical inference from the first principles of the studied subject.

255   **RESULTS AND DISCUSSION**

256   According to Alexander Watt, a a plant ecosystem may be considered '*as a working mechanism*'
257   which '*maintains and regenerates itself'* (Watt 1947). Our model demonstrates a such
258   mechanism. From a more general physical point of view we model an active (excitable) media
259   with autowaves (travelling waves, self-sustaining waves) (Kalmykov & Kalmykov 2013; Krinsky
260   1984; Zaikin & Zhabotinsky 1970). Active medium is a medium that contains distributed
261   resources for maintenance of autowave propagation. An autowave is a self-organizing and self-
262   sustaining dissipative structure. An active medium may be capable to regenerate its properties
263   after local dissipation of resources. In our model, propagation of individuals occurs in the form of
264   population waves. We use the axiomatic formalism of Wiener and Rosenblueth for modeling of
265   excitation propagation in active media (Wiener & Rosenblueth 1946). In accordance with this
266   formalism rest, excitation and refractoriness are the three successive states. In our formalism the
267   rest state corresponds to the free state of a microhabitat, the excitation state corresponds to the
268   life activity of an individual in a microhabitat and the refractory state corresponds to the
269   regeneration state of a microhabitat. All states have identical duration. If the refractory period
270   will be much longer than the active period, then such a model may be interpreted, for example, as
271   propagation of the single wave of dry grass fire. Time duration of the basic states can be easily
272   varied using additional states of the lattice sites.
273   Different initial conditions may lead to formation of different spatio-temporal patterns and as a
274   result they may lead to different dynamics of the system. Using the Monte Carlo method, we
275   have investigated the influence of different initial conditions on population dynamics of one
276   species. We have investigated two different boundary conditions, two different cellular automata
277   neighborhoods and four different lattice sizes (Figs 5 and 6). Ecosystem dynamics on the plane
278   with boundary is more natural than on a torus, where boundary effects are absent. The models
279   with non-periodic boundary conditions correspond to laboratory and field experiments where
280   experimental plots also have a boundary. Models with periodic boundary conditions are
281   investigated more commonly, as they allow to avoid boundary effects. Periodic boundary
282   conditions cannot be reproduced in real ecosystems, but they allow to investigate models in a
283   more general form. Therefore, we decided to explore the both types of boundary conditions.
284   Figure 5 shows the results obtained in the study of aggressive propagation and Figure 6 shows the
285   results obtained in the study of moderate propagation. In Figs 5B-D and 6E-H we show the S-
286   shaped population growth and in Fig. 6B-D we show the double S-shaped population growth.
287   Sizes of the lattice which define available space for colonization consisted of 3x3, 8x8, 23x23
288   and 98x98 sites. We have investigated the boundary conditions of two types - when the lattice
289   was closed on the torus by periodic conditions (Fig 5A-D and Fig 6A-D) and when the lattice has
290   a boundary (Fig 5E-H and Fig 6E-H). There were no changes of population dynamics in result of
291   the different initial positioning of an individual on the lattice in cases with periodic boundary
292   conditions (Fig 5A-D and Fig 6A-D). In cases when a lattice has a boundary, different initial

293 positioning of an individual lead to differences in population dynamics (Fig 5E-H and Fig 6E-H).
294 Moreover, increasing of the lattice may lead to more complex dynamics (Figs 5E-H, 6E-H).
295 Periodic fluctuations in numbers of individuals are observed at the plateau phase in most of the
296 experiments. With increasing of the lattice size, these periodic fluctuations in population size
297 become less visible. The periodic fluctuations on the plateau phase are absent when the lattice
298 consists of 3x3 sites in the case of the tripod neighborhood (Fig. 6A, 6E). The similar plateau
299 phases without fluctuations were found at the 3Nx3N sizes of the lattice (6x6, 9x9, 12x12, 15x15,
300 18x18, 27x27 lattices were tested), with and without boundary effects and when the
301 neighborhood was tripod.

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

308 We show four Movies S1-S4 As examples of the Monte Carlo simulations. Each Monte Carlo
309 simulation consists of five repeated experiments with different initial positioning of an individual
310 on the lattice. The lattices are homogeneous and limited in all experiments. They are consisted of
311 23x23 sites available for occupation by individuals. In Movie S1 the lattice is closed on the torus
312 and the neighborhood is hexagonal. In Movie S2 the lattice has a boundary and the neighborhood
313 is hexagonal. In Movie S3 the lattice is closed on the torus and the neighborhood is tripod. In
314 Movie S4 the lattice has a boundary and the neighborhood is tripod.

Without edge effects (torus-lattice)
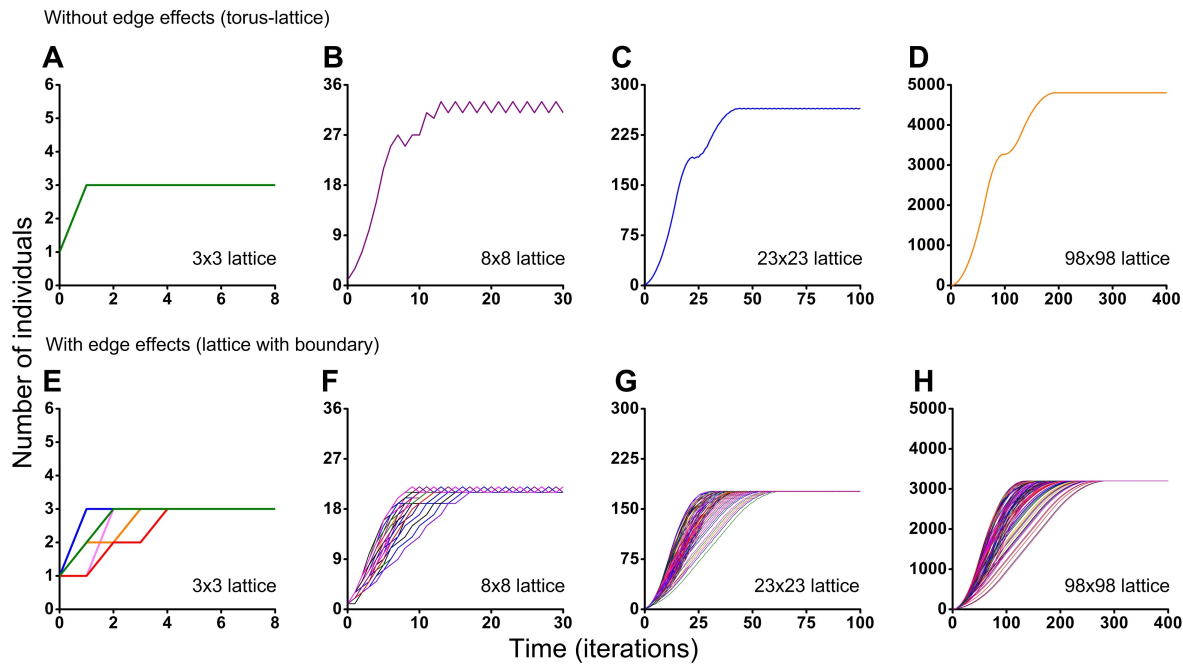
With edge effects (lattice with boundary)

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

In more detail individual-based mechanisms of the double S-shaped population growth curve are presented in Fig. 7C and Movie S7. Details of individual-based mechanisms of three types of the S-shaped population growth curves are presented in Fig. 7A, 7B, 7D and in Movies S5, S6, S8.

333 Figure 7A shows the S-shaped population growth curve with short phase of decelerating growth.
334 This curve reaches a plateau earlier than on population curves in Figures 7B-D. The plateau is
335 reached on the 32nd iteration (Movie S5). The higher rate of population growth is explained by
336 aggressive propagation and by the lack of boundary effects because the lattice of closed into a
337 torus.
338 Figure 7B shows the S-shaped population growth curve with sharp transition to long phase of
339 decelerating growth. This curve has a sharp slowdown of population growth before the beginning
340 of phase of decelerating growth. It occurs on the 25th iteration, when population waves of
341 aggressively propagating species reach the habitat boundary (Movie S6). In contrast to the curve
342 in Figure 7A, this population curve reaches the plateau on the 49th iteration. Reduced population

343   growth rate of aggressively propagating species is explained by the presence of boundary effects
344   because the lattice has a boundary.
345   In Figure 7C the population growth curve has a double S-shaped form. The double S-shaped
346   population growth is a result of temporary slowdown of growth, which occurs at the stage when
347   colonization of the free field is replaced by interpenetration of colliding population waves into
348   already occupied areas. Starting from the 34th iteration, the stage of gradually compaction of
349   populated areas begins (Movie S7). This compaction arises from the fact that after rounding of
350   the torus population waves occupy the remaining free sites in the partially populated part of
351   habitat as result of a 'phase shift' of the colliding waves. The free vacancies in population waves
352   remain in result of moderate propagation of individuals. The moderate propagation is modeled by
353   the tripod neighborhood. Speed of the sealing colonization increases slowly due to the form of
354   the population waves which invade into already occupied areas by the expanding wedge. At the
355   same time contribution into population growth from colonization of the areas which consists only
356   of free sites (microhabitats) decreases. The areas which consist only of free microhabitats
357   disappear on the 49th iteration. The population growth rate temporarily slows down what forms
358   the first plateau of the curve. This plateau phase lasts during 5 iterations. The accelerating of
359   additional compactization of population waves leads to the new population growth starting from
360   the 53rd iteration. The population curve reaches the second plateau on the 98th iteration.
361   Figure 7D shows the S-shaped population growth curve with very long phase of decelerating
362   growth. This curve reaches a plateau on the 72nd iteration (Movie S8). Reduced population
363   growth rate and reduced maximum number of individuals in the habitat (834 individuals) are a
364   result of the boundary conditions and the moderate fecundity of individuals (because of tripod
365   neighborhood).

366   **The S-shaped and the J-shaped population growth curves**
367   We have investigated the S-shaped population growth which is limited by following factors:
368   finite size of the habitat (limited resources), habitats' size, type of boundary conditions of habitat,
369   intraspecific competition, lifetime of individuals, regeneration time of microhabitats, fecundity of
370   individuals (Figs 2, 5-7 and Movies S1-S8). In this section we show the model of the J-shaped
371   population growth and investigate two cases of geometric population growth. Unlike of the S-
372   shaped population model, the J-shaped population model describes a situation in which
373   population growth is not limited in resources, by intraspecific competition or for any other
374   environmental reasons. J-shaped population model describes a full reproductive potential which
375   lead to geometrical population growth (Fig. 8). In other respects this model similar to our model
376   of the S-shaped population growth. It also takes into account natural decline of individuals.
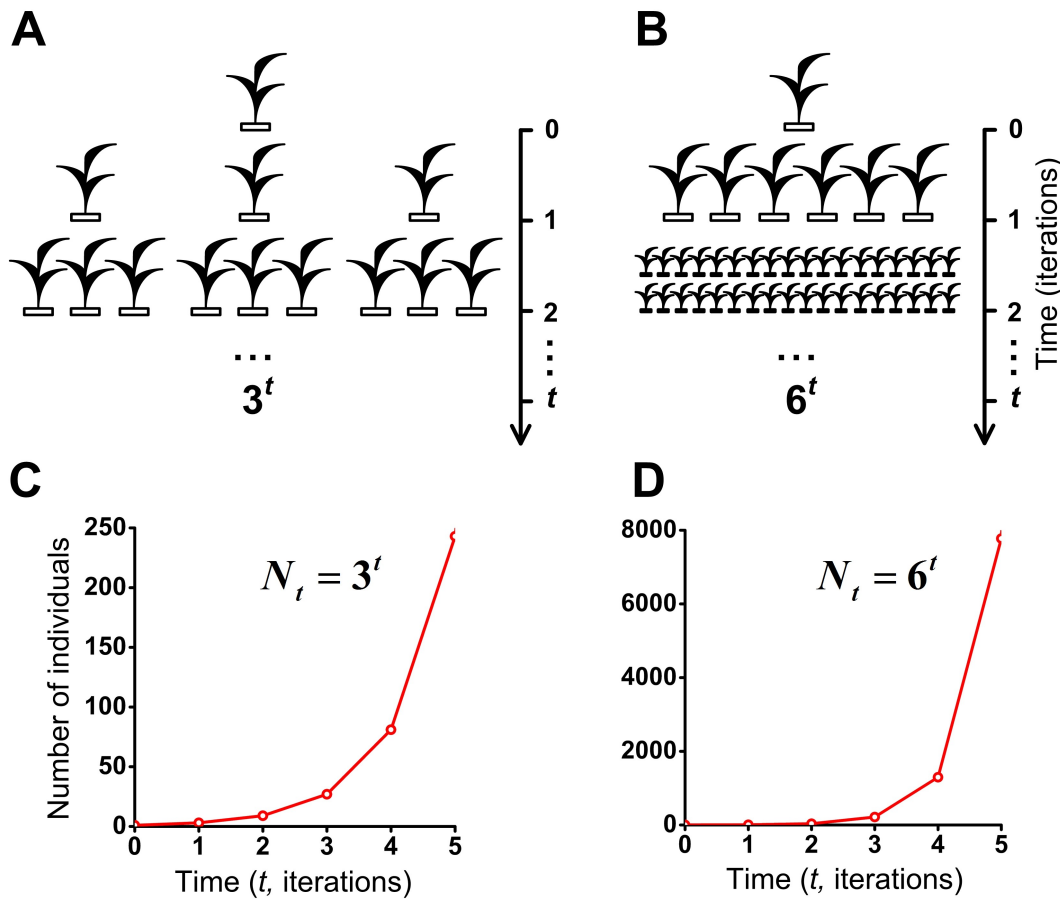377   Individual's lifetime equals one iteration.

Figure 8: J-shaped population growth. 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 have compared our model of the S-shaped (Fig. 7A and Movie S5) with the J-shaped population growth (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 the S-shaped and the double S-shaped population growth with the J-shaped population growth.

392 **Table 1: Comparative population dynamics in the models with the S-shaped and**
393 **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

394 **Table 2: Comparative population dynamics in the models with the double S-**
395 **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

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

CONCLUSIONS

We have presented and investigated a mechanistic model of dynamics of single species plant population. This model is based on pure logical deterministic individual-based cellular automata. It has a physical and ecological ontology. Here the physical ontology is the ontology of the active medium and ecological ontology represents an ecosytem with one vegetatively propagated plant species. We investigated deterministic individual-based mechanisms underlying the S-shaped and double S-shaped population growth of vegetatively propagated plants. Iimitating modeling of vegetatively propagated rhizomatous lawn grasses was not our main goal. The main goal was demonstration of possibilities of the white-box modeling on example of population growth. The white-box model was made on the basis of physical axioms of excitation propagation in excitable medium. These basic physical axioms of the model have a universal character that, in principle, allows transferring the obtained results to other subject areas. An additional important result is itself demonstration of the white-box modeling of complex systems using logical cellular automata. We consider the details of the "white-box modeling" methodology as the main results of our work. We would like to make this perspective approach more widely used in the practice of mathematical modeling of complex systems. And we have tried to supplement the discussion about "the value of white boxes" by considering specific ways of implementation this model approach. Our study directly introduces the white-box approach into ecological modeling. The white-box approach opens up new perspectives in modeling by implementing a multy-level mechanistic modeling of complex systems. Our deterministic logical cellular automata model works as a system of artificial intelligence. Cellular automata are known as the method of artificial intelligence. But there is a problem how to use this method of artificial intelligence for investigation of complex systems. We show how logical deterministic cellular automata may be used for mathematical white-box modeling of complex systems on example of ecosystem with one species. Parallelism of the logical operations of cellular automata in total volume of the modeled macrosystem allows to speak that the model hyper-logically provides automatic deductive inference. The term 'deductive' is used here because all logical operations are based on axioms. We consider that the main difficulty of this white-box modeling is to create an adequate axiomatic system based on an intrinsic physical ontology of the complex system under study. The main feature of the approach is the use of cellular automata as a way of linking semantics (ontology) and logic of the subject area. Our logical white-box model of an ecosystem with one species combines reductionist and holistic approaches to modeling of complex systems. We consider the white-box modeling by logical deterministic cellular automata as a perspective way for investigation of any complex systems.

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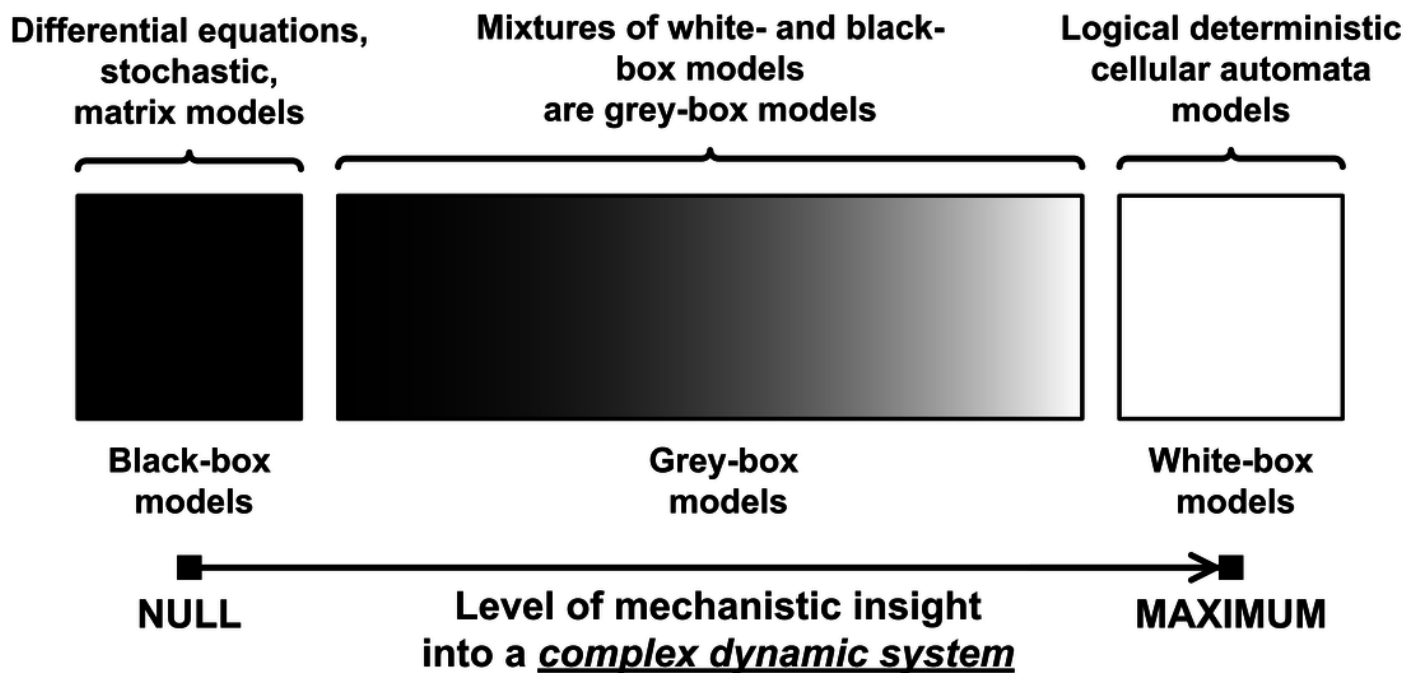
440 **REFERENCES**

441 Anonymous. 1944. British Ecological Society. Easter meeting 1944: Symposium on "The Ecology of Closely Allied
442   Species." *Journal of Animal Ecology* 13:176-177. doi: http://www.jstor.org/stable/1450?origin=JSTOR-pdf

443 Clark JS. 2009. Beyond neutral science. *Trends in Ecology & Evolution* 24:8-15. doi: 10.1016/j.tree.2008.09.004

444 Craze P. 2012. Ecological neutral theory: useful model or statement of ignorance? *Cell Press Discussions*. URL:
445   http://news.cell.com/discussions/trends-in-ecology-and-evolution/ecological-neutral-theory-useful-model-
446   or-statement-of-ignorance

447 Grubb PJ. 1977. The maintenance of species-richness in plant communities: the importance of the regeneration
448   niche. *Biological Reviews* 52:107-145. doi: http://dx.doi.org/10.1111/j.1469-185X.1977.tb01347.x

449 Hubbell SP. 2001. *The unified neutral theory of biodiversity and biogeography*. Princeton, N.J. ; Oxford: Princeton
450   University Press.

451 Huston M, DeAngelis D, and Post W. 1988. New Computer Models Unify Ecological Theory. *Bioscience* 38:682-
452   691. URL: http://www.jstor.org/stable/1310870

453 Kalmykov LV, and Kalmykov VL. 2011. Deterministic individual-based cellular automata modelling of single
454   species population dynamics. *Available from Nature Precedings*:1-15. doi:
455   http://dx.doi.org/10.1038/npre.2011.6661.1

456 Kalmykov LV, and Kalmykov VL. 2012. Mechanistic mechanisms of competition and biodiversity. *Available from
457   Nature Precedings*:1-34. doi: http://hdl.handle.net/10101/npre.2012.7105.1

458 Kalmykov LV, and Kalmykov VL. 2013. Verification and reformulation of the competitive exclusion principle.
459   *Chaos, Solitons & Fractals* 56:124-131. doi: http://dx.doi.org/10.1016/j.chaos.2013.07.006

460 Komarov AS, Palenova MM, and Smirnova OV. 2003. The concept of discrete description of plant ontogenesis and
461   cellular automata models of plant populations. Ecological Modelling 170:427-439. doi:
462   http://dx.doi.org/10.1016/S0304-3800(03)00243-6

463 Krinsky VI. 1984. Autowaves: Results, problems, outlooks. In: Krinsky VI, ed. *Autowaves: Results, problems,
464   outlooks in Self-Organization: Autowaves and Structures Far from Equilibrium* Berlin: Springer-Verlag, 9-
465   19.

466 Rosindell J, Hubbell SP, He F, Harmon LJ, and Etienne RS. 2012. The case for ecological neutral theory. *Trends in
467   Ecology & Evolution* 27:203-208. doi: http://dx.doi.org/10.1016/j.tree.2012.01.004

468 Silvertown J, Holtier S, Johnson J, and Dale P. 1992. Cellular Automaton Models of Interspecific Competition for
469   Space - the Effect of Pattern on Process. *Journal of Ecology* 80:527-534. URL:
470   http://www.jstor.org/stable/2260696

471 Sommer U. 1999. Ecology - Competition and coexistence. *Nature* 402:366-367. doi: http://dx.doi.org/10.1038/46453

472 Tilman D. 1987. The importance of the mechanisms of interspecific competition. *The American Naturalist* 129:769-
473   774. doi: http://dx.doi.org/10.1086/284672

474 Watt AS. 1947. Pattern and Process in the Plant Community. *Journal of Ecology* 35:1-22. doi:
475   http://dx.doi.org/10.2307/2256497

476   Wiener N, and Rosenblueth A. 1946. The mathematical formulation of the problem of conduction of impulses in a
477   network of connected excitable elements, specifically in cardiac muscle. *Arch Inst Cardiol Mex* 16:205-265.
478   Zaikin AN, and Zhabotinsky AM. 1970. Concentration Wave Propagation in Two-dimensional Liquid-phase Self-
479   oscillating System. *Nature* 225:535-537. doi: http://dx.doi.org/10.1038/225535b0

1

Three types of mathematical models for complex dynamic systems.

This is a schematic representation of a black-box model, a grey-box model and a white-box model with the level of their mechanistic understanding.

Differential equations, stochastic, matrix models **Mixtures of white- and black-box models are grey-box models** **Logical deterministic cellular automata models**

Black-box models **Grey-box models** **White-box models**

NULL **Level of mechanistic insight into a _complex dynamic system_** MAXIMUM

2

S-shaped population growth.

A logical deterministic individual-based cellular automata model of an ecosystem with one species shows both population dynamics and pattern formation. The lattice consists of 25x25 sites. Individuals use the hexagonal neighborhood for propagation. The lattice is closed on the torus to avoid boundary effects. (**A-C**) Population dynamics of the species. S-shaped population growth curve (C). (**D-F**) Spatio-temporal patterns of the model represented in numerical form of program implementation.

3

Cellular automata neighborhoods.

A cellular automata neighborhood models a vegetative propagation of plants and defines fecundity and spatial positioning of an individual's offsprings. Positioning of offsprings is explained by how the cellular automata neighborhood is implemented successively for each lattice site. A central site of the neighborhood is defined by the array element with index (i, j), where i and j are integer numbers. Neighboring sites of the central site are defined by the array elements with indexes. (**A**) Hexagonal neighborhood. (**B**) A model example of vegetative propagation of an individual in the hexagonal neighborhood. Offsprings occupy all nearest lattice sites what corresponds to aggressive propagation. A maximum number of offsprings per one individual (fecundity) equals six. (**C**) Tripod neighborhood. (**D**) A model example of vegetative propagation of an individual in the tripod neighborhood. Offsprings occupy a half of the nearest lattice sites what corresponds to the moderate propagation. A maximum number of offsprings per one individual equals three.
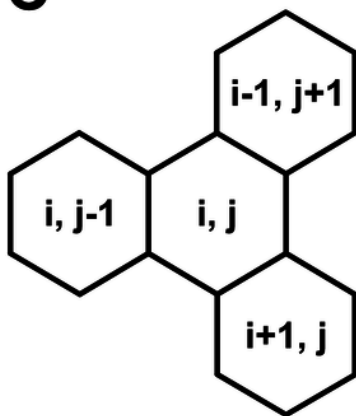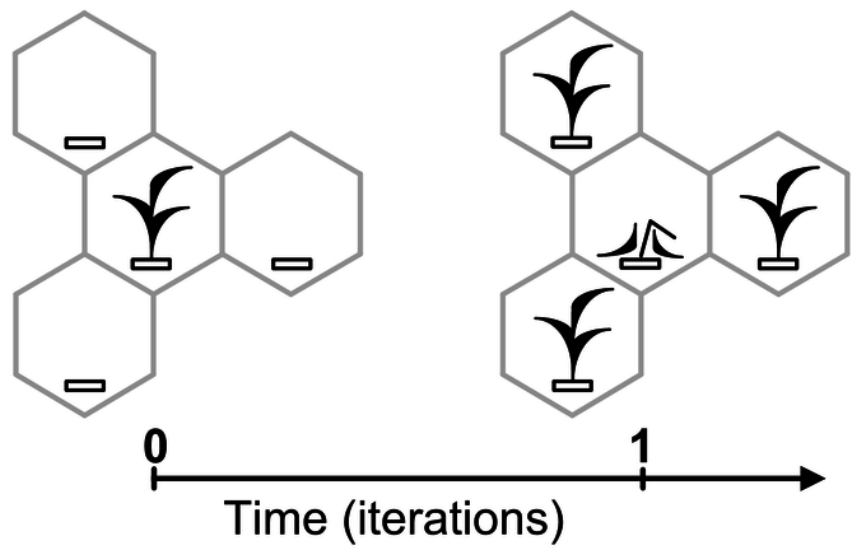
A

i-1, j i-1, j+1

i, j-1 i, j i, j+1

i+1, j-1 i+1, j

B

0   1

C

i-1, j+1
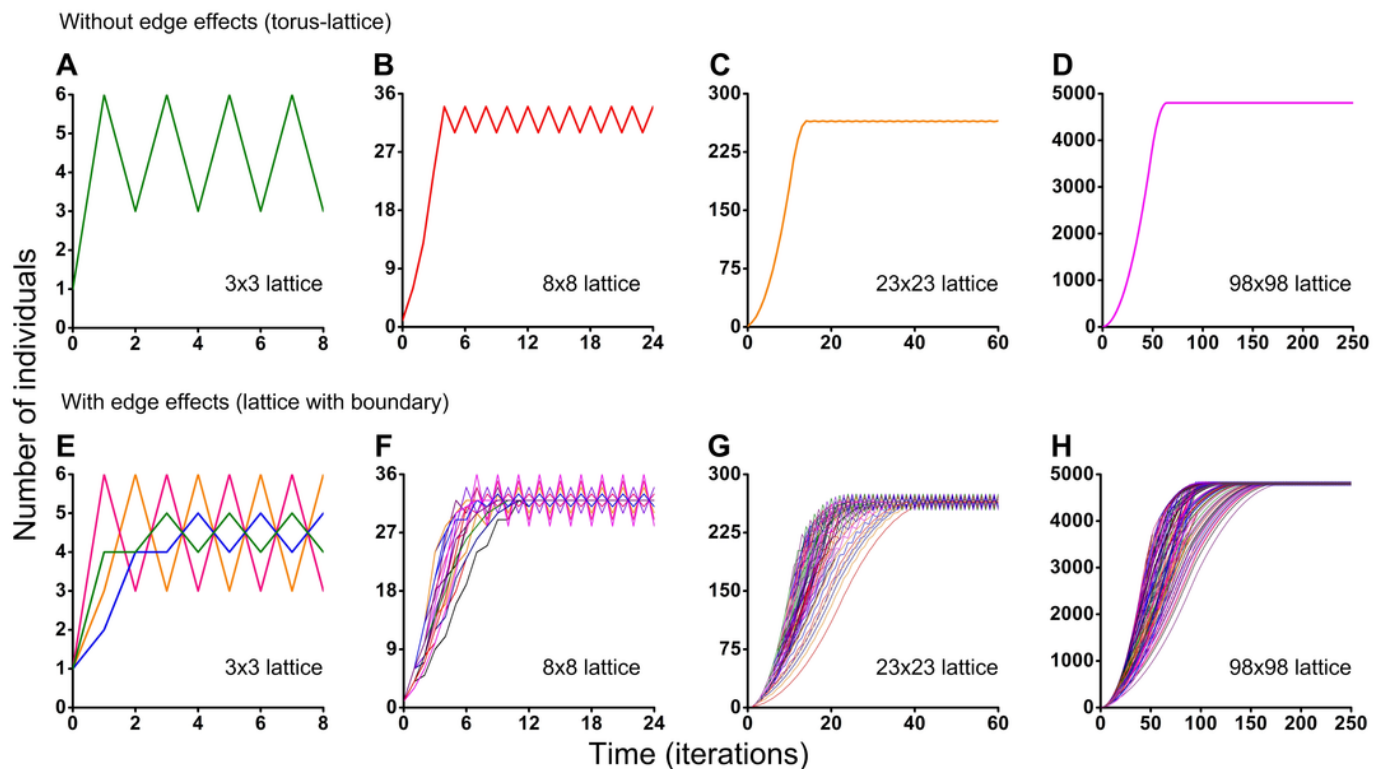
i, j-1 i, j

i+1, j

D

0   1

Time (iterations)

4

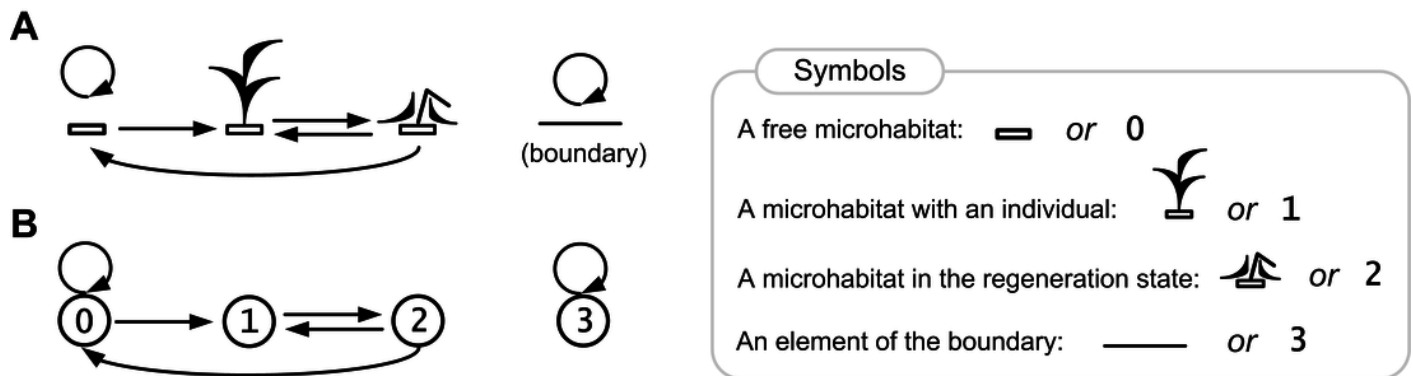Results of the Monte Carlo simulations with the hexagonal neighborhood.

Investigation of the influence of boundary conditions, initial positioning of an individual and lattice sizes on single-species population dynamics. (**A-D**) The lattice is closed on the torus to avoid boundary effects. (**E-H**) The lattice has a boundary. Every Monte Carlo simulation consisted of 100 repeated experiments with different initial positioning of an individual on the lattice.

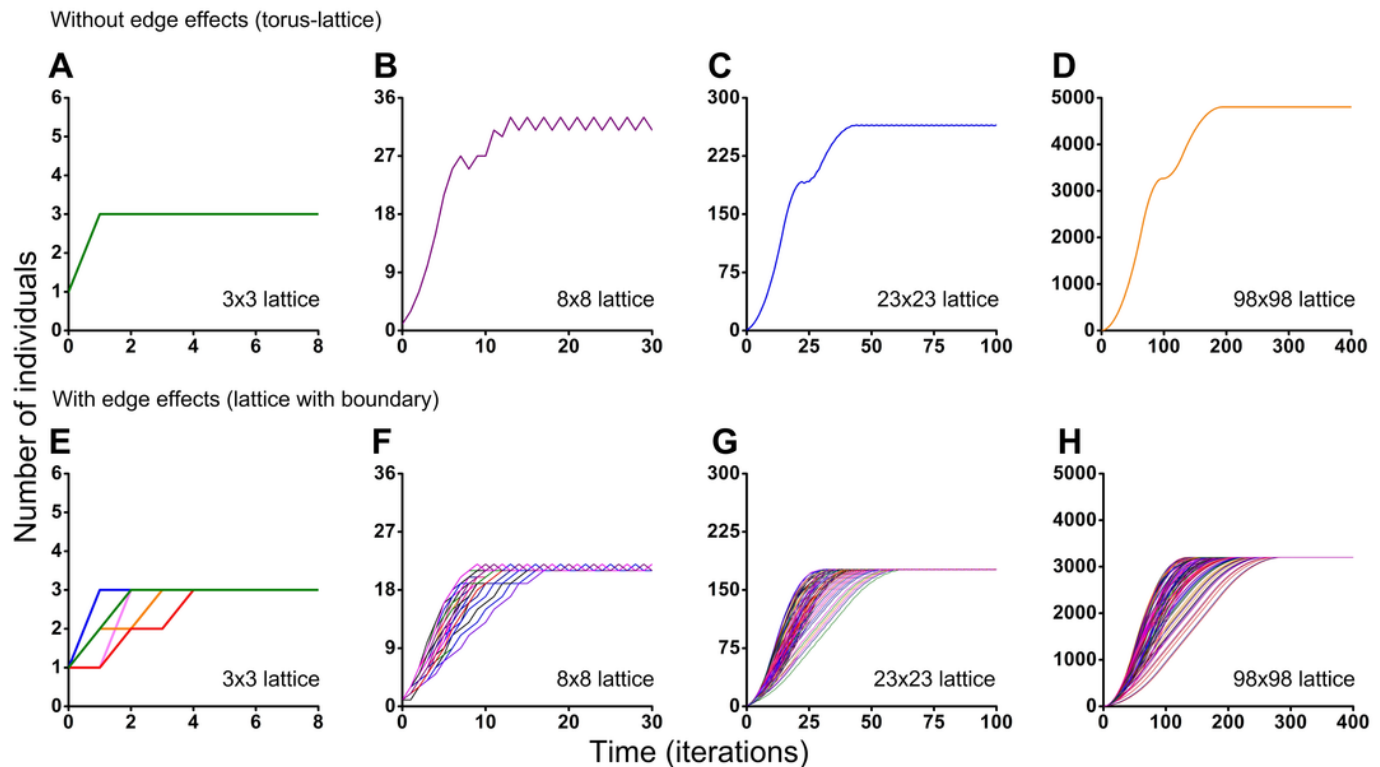5

Rules of the ecosystem model with one species.

Directed graph of transitions between the states of a lattice site is represented in pictorial (A) and numerical forms (B). The graph represents a birth-death-regeneration process.

6

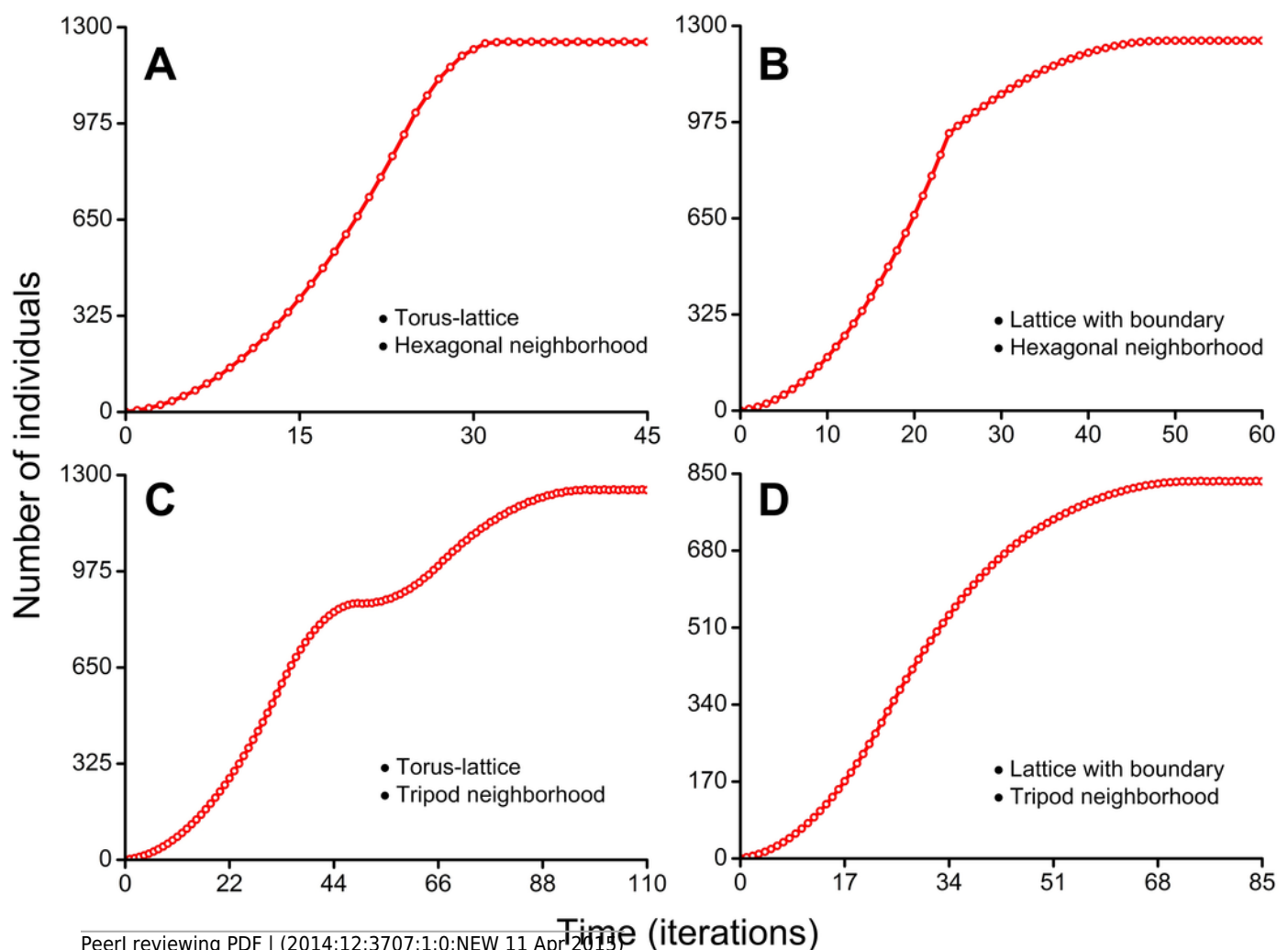Results of the Monte Carlo simulations with the tripod neighborhood.

Investigation of the influence of boundary conditions, initial positioning of an individual and lattice sizes on single-species population dynamics. (**A-D**) The lattice is closed on the torus to avoid boundary effects. (**E-H**) The lattice has a boundary. Every Monte Carlo simulation consisted of 100 repeated experiments with different initial positioning of an individual on the lattice.

7

Population growth curves.

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

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).

A

3^t

B

6^t

Time (iterations)

C

$N_t = 3^t$

Number of individuals

Time (*t*, iterations)

D
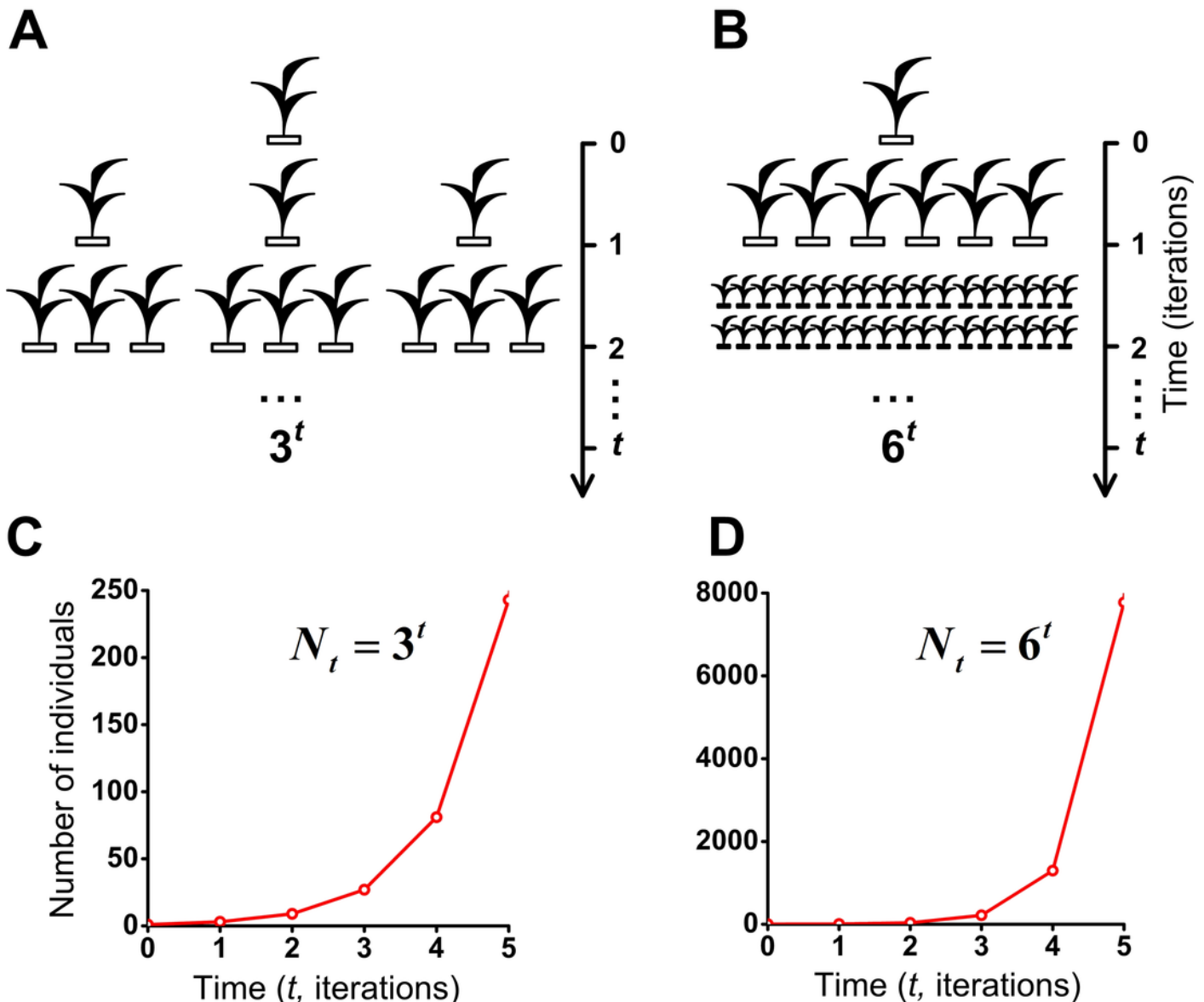
$N_t = 6^t$

Time (*t*, iterations)

Table 1(on next page)

Comparative population dynamics in the models with the S-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. 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

Table 2(on next page)

Comparative population dynamics in the models with the double S-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