

Simulation as a Tool to Identify Dynamical Typology of Water Frog Hemiclonal Population Systems

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Abstract. Some related species give rise to interspecies hybrids with hemiclonal inheritance. The gametes of such hybrids transfer the set of hereditary information of one of the parental species. The water frog, *Pelophylax esculentus*, is an example of such hybrids. The hemiclonal hybrids together with their parental species form a biosystem for which the suggested name is Hemiclonal Population System (HPS). The phenomenon of interspecific hemiclonal reproduction of water frogs has been intensively explored for several decades, but insufficient study has been devoted to the mechanisms of the composition constancy and ecological stability of their population systems.

In this paper we focus on sustainability and possible results of transformations (in terms of different genetic forms and of population dynamics of each of these forms) of HPSs that consist of diploid representatives. By means of a simulation model we evaluated the long-term consequences of parameters that were derived from empirical research on a natural HPS at a particular brief time-period. This research was carried out in the region of eastern Ukraine, the so-called Siverskyi Donets center of diversity of the *Pelophylax esculentus* complex. Our study describes the development of a dynamic typology of the HPS by principal component analysis of data generated by the simulations. We investigate the space of the possible states of the HPS. The simulations helped to split this state-space into six areas of stability, each of which corresponds to a different type of stability. Before conducting the simulation study we assumed there were only four truly stable states. Two new states were identified as a result of using this model.

Keywords: Dynamic Typology, Hemiclonal Inheritance, *Pelophylax esculentus* complex, Simulation Modelling.

1 Introduction

1.1 Motivation

The processes of transformation of natural biological systems (populations, ecosystems etc.) are an important challenge for modern science. In many cases these processes are not readily available for direct study (e.g. because of their long duration). In such cases we have to reconstruct their transformation models based on (1) the observed diversity of their natural states, (2) our hypothesis of what controls the change of such states, and (3) available empirical data. A simulation model plays a key role in such studies. Thanks to it, we can determine the possible directions of transformation of the target systems and build their typology. One of the insufficiently studied types of biological systems are those that create species capable of interspecies hybridization and their hemiclinal hybrids. Reproduction of hemiclinal hybrids occurs in biological systems which have been described as Hemiclinal Population Systems (HPSs) [15]. Water frogs are a typical model organism for studying such systems.

This paper describes a computer simulation study of Hemiclinal Population Systems (HPS) of water frogs. First we introduce the peculiar characteristics of these biosystems. In the next section we indicate the advantages of computer simulation as a modelling tool together with the specific characteristics of the model presented here. Computer simulation has been described as the collaboration between experimenting and modelling [7]. The existing empirical data was used to determine model parameters and to assess the performance of the model against real-world situations. We describe experiments conducted upon the model itself and the way in which these can supplement fieldwork findings.

1.2 Reproduction within HPSs

Most life forms which arise from sexual reproduction exhibit the typical biosystem hierarchy in which organisms exist as part of populations that form species. In these populations, genetically unique individuals produce sex cells (gametes), which bear a unique genome (holistic unitary complex of hereditary information) resulting from recombination of two parental genomes (Fig.1 A). The consequence of this is the existence of a population gene pool (common pool of genes). Populations of organisms with clonal reproduction, on the other hand, consist of clones, i.e. sets of genetically identical organisms (with accuracy limited by the error rate of copying during reproduction). These populations are presented as a set of relatively isolated lines consisting of genetically identical maternal and child individuals.

This work is dedicated to a relatively rare type of population reproduction which differs from the two mentioned options. It is characteristic of hybridogenic complexes of species. This complex consists of two parental frog species [11]. Their full zoological names are *Pelophylax lessonae* (Camerano, 1882) and *Pelophylax ridibundus* (Pallas, 1771). They cross to produce hybrids named analogous to the species' name, e.g. *Pelophylax esculentus* (Linnaeus, 1758).

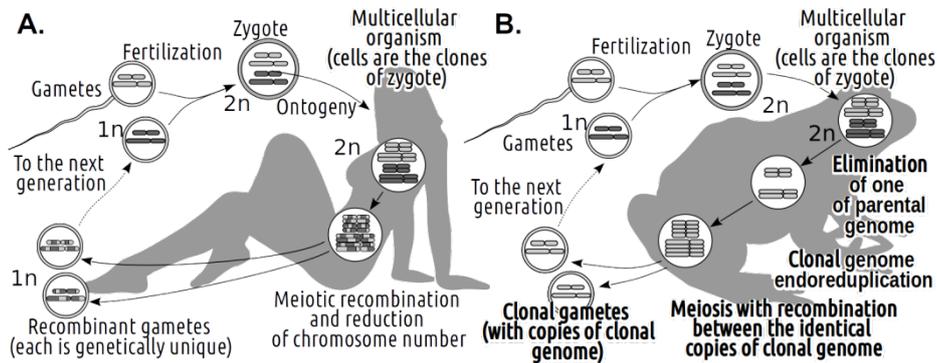


Fig. 1. A comparison of the life cycle with fertilization and meiosis, which is characteristic of organisms with sexual reproduction (A), and modification of such a cycle, which is characteristic of interspecific hybrids with hemiclonal inheritance (B).

The differences between the genomes of the parental species lead to the fact that production of normal gametes through recombination becomes impossible. Breeding hybrids is made possible by specific changes in their life cycle (Fig. 1B). One parent genome of such hybrids is eliminated from the germline cells (i.e. those cells which subsequently form the sex cells, gametes). Thereafter, the second parental genome undergoes endoreduplication (i.e. doubles without cell division). This gives rise to cells with two genomes that are identical (with accuracy limited by the errors of copying). They form genetically identical gametes.

Hemiclonal hybrids differ both from usual organisms with recombinant reproduction and from clonal organisms. A HPS, where hemiclonal hybrids are reproduced, differs from normal recombinant and from clonal populations. The features of a HPS are as follows [15]:

- Cooperative reproduction of individuals that differ in species composition of their genomes (i.e. representatives of parental species and hybrids of various genome compositions);
- Vertical transmission of the clonal genome lines, which can combine with other recombinant or clonal genomes;
- In the HPS, which includes individuals of the parental species, these individuals support the existence of a pool of recombining genes (gene pool), which corresponds to the gene pool of conventional monospecific populations;
- Cases of limited interspecies recombination are observed (i.e. transferring of fragments of genetic information from the genome of one parental species into the gene pool of another parental species).

The most common typology of a HPS is associated with an indication of the parental species and diploid hybrids and/or triploid hybrids, which are included in their composition. The presence of *P. esculentus* is indicated by the letter **E**, letter **L** stands for *P. lessonae*, and letter **R** for *P. ridibundus*. The presence of polyplod *P. esculentus* is

denoted by the letter **p**. Thus, L-E-HPS consists of *P. lessonae* and diploid *P. esculentus*, and R-E-HPS consists of *P. ridibundus* and diploid *P. esculentus*. Clonality of a genome is designated by putting its symbol in brackets. The water frogs' sex determination system is similar to that in humans. The structure of the female genome includes the sex chromosome X. Individuals that have two female genomes are female (♀). The structure of the male genome includes the sex chromosome Y. Individuals with one female and one male genome are male (♂).

Consider the simplest example of a L-E-HPS (Fig. 2), which includes a parent species (*P. lessonae*) as well as hybrids which clonally transmit the female *P. ridibundus* genome (^XR). Hybrids are reproduced when crossed with the parental species individuals: ♀^XL(^XR) × ♂^XL^YL → ♀^XL(^XR) : ♂^YL(^XR); ♀^XL^XL × ♂^YL(^XR) → ♀^XL(^XR).

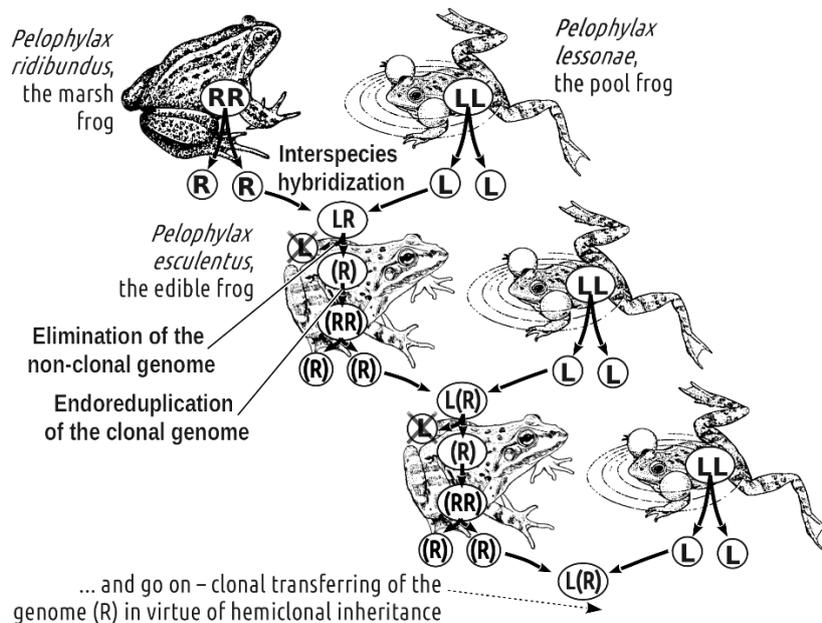


Fig. 2. The occurrence of *Pelophylax esculentus* due to hybridization of *Pelophylax lessonae* with *Pelophylax ridibundus* and reproduction of *P. esculentus* with the parental species in L-E-HPS.

Different regions of the *P. esculentus* complex distribution are characterized by HPSs of various compositions [2, 10, 11]. In some regions there are *P. esculentus* individuals which simultaneously produce gametes (L) and (R). This phenomenon is called hybrid amphisperry. Such individuals are referred as (L)(R).

By crossing hybrids, which transmit genomes of the same parental species, there may occur representatives of these species. Typically, these individuals die before sexual maturity: ♀^XL(^XR) × ♂^YL(^XR) → ♀^XR^XR → †.

Different forms of frogs in a HPS differ in their vitality and fertility. The composition of zygotes, tadpoles and frogs of the different ages in the same HPS may vary significantly. Another feature of the hybridogenic complex of water frogs (not considered in

this study) is that in some regions there are not only diploid hybrids (i.e., having two genomes), but hybrids with three (LLR or LRR) and even four (e.g. LLRR) genomes [2, 15].

Hemiclonal hybridization, the consequence of which is the occurrence of a HPS, is observed not only for the water frogs, but also for some other species groups [1].

HPSs of hybridogenic species complexes are a little-known category of biosystems. Their study, part of which is a simulation of their transformations, should lead to important results. For example, the particular genome-selective elimination in interspecific hybrids may open new opportunities in biotechnology and genetic medicine. This allows, if necessary, the removal of unwanted fragments of the genome. Hemiclonal inheritance supports all offspring from crossing of two individuals (each of which transmits a clonal genome) to be genetically identical, i.e. clonal. The resulting organisms, which inherit clonal genomes of two different parent species, may be useful for biotechnology and agriculture. Study of the reason of the hemiclonal hybridization occurrence and the effects of this phenomenon on the evolution of hybridizing species are of considerable theoretical interest. Although study of HPS transformations per se cannot solve these problems, it allows one to better understand mechanisms of appearance and maintenance of the stability of a biological system in which such amazing genetic phenomena are possible.

For further study, it is necessary to describe the variety of possible states of HPSs, their dynamics, regularities and the conditions under which they are stable.

Direct study of HPSs faces significant challenges. Determination of their composition and reproduction mechanisms is associated with a significant amount of fieldwork. HPSs are relatively unusual and differ from well known biosystems such as biocenoses and sexually or clonally reproducing populations. Processes of change in HPS are quite extended temporally and may take decades. There is a high degree of variability in the composition of different HPSs and some are unique objects whose occurrence is highly unlikely. The study of only one unique HPS may not be enough for understanding the regularities of their dynamics. Additionally, HPSs are complex systems containing many stochastically interacting components.

Some authors have used analytical modelling to describe the dynamics of a population system of water frogs [14, etc.]. Analytical models are suitable for the study of separate aspects of the HPS dynamics, however their usage faces significant challenges due to fact that a HPS is governed by an interrelated set of stochastic processes. We therefore consider simulation to be a more useful tool to study the general properties of HPSs.

Christiansen [4] simulated reproduction of *P. esculentus*. Christiansen's model is deterministic whereas our model allows modelling of random events in competition and breeding of animals. The works of Bove et al. [3] and Quilodran et al. [12] are recent studies based on the simulation of water frogs' HPSs. These studies consider the stability of specific types of HPSs under certain conditions. Our work, in contrast, seeks to analyze all possible stable states of a certain category of HPSs.

Differences of our simulation from others are as follows. At the same time, we consider typical for most populations demographic factors (non-competitive and competitive mortality, differences in the reproduction probability, changes in viability with age)

and the unique features of HPS. Our work considers the entire space of possible states of a certain category of HPS. Finally, we use population parameters, the estimates of which were obtained during field studies of this category of HPS.

1.3 Scope of Modelling

Several authors of this work have previously built a deterministic discrete-time simulation model [5]. It enabled investigators to determine the population composition for a specified number of simulation steps, commencing with the current HPS composition. The objective of the current work is identification of the set of stable states of a HPS (consisting solely of diploid water frog individuals) using a stochastic simulation.

The research was conducted in two stages. In the first stage a number of simulation experiments were performed for various initial compositions of the model HPS. The aim of this stage was to get insight into the possible end states for the HPSs. The second stage analyzed and classified these end states. The dynamic typology of the system was constructed based on the various initial compositions of the HPSs, the observed final states, and the observed transitions from initial to final states.

Dynamic typology is based not only on analysis of the observed object states, but, above all, on a forecast of their future dynamics [9]. In this respect, dynamic typology differs both from associative typology (identification of groups of objects, related to one or more samples) and from analytical typology (partitioning of a set of objects into groups depending on the state of their observable characteristics) [15].

Hybrid frogs are reproduced differently in different regions [10, 14]. Before the problem of the dynamical typology is solved in general, for all possible types of HPSs and all known genetic forms of hybrids and their reproduction, it should be solved for one selected region. Authors of the current paper have previously described the Siverskyi Donets center of diversity of the *Pelophylax esculentus* complex located at the eastern Ukraine [15]. It is characterized by a high diversity of HPSs and provides the potential to test the adequacy of the model. The distribution of HPSs, including polyploid hybrids (not discussed in this paper), is related to the flood plain of the river Siverskyi Donets, and to its small tributaries and ponds located nearby within the Kharkiv and Donetsk regions. Within the Mzha and the Uda river basins (right tributaries of the Siverskyi Donets), HPSs consisting exclusively of diploids are widespread. The nature of gamete production in diploids from the Siverskyi Donets and Mzha and the Uda river basins is similar.

We plan to describe the total variety of HPSs from the Siverskyi Donets center of diversity of the *Pelophylax esculentus* complex. As the first step, we consider a variety of HPSs located in the Mzha and the Uda river basins which consist of diploid representatives.

2 Model Description and its Justification

2.1 The Cycle of the Model

A simulation model, as opposed to an analytical model, describes the process of the state transformations during time, not the dependence of the future states of the system on the current one. Therefore, for model development it is sufficient to describe the algorithm of changes in the HPS sizes with time. In this model, time is divided into discrete steps through which the model cycles. The cycle of the model corresponds to the calendar year. It sets the sequence of transformations: ${}^a\mathbf{n}^g_a \rightarrow \beta\mathbf{n}^g_a \rightarrow \gamma\mathbf{n}^g_a \rightarrow \delta\mathbf{n}^g_a \rightarrow \omega\mathbf{n}^g_a$. Here ${}^a\mathbf{n}^g_a$, $\beta\mathbf{n}^g_a$, $\gamma\mathbf{n}^g_a$, $\delta\mathbf{n}^g_a$ and $\omega\mathbf{n}^g_a$ is a sequence of transformations of the individual's groups of the genotype (\mathbf{g}) and of the age (\mathbf{a}) which correspond to the different stages of the annual cycle (Table 1).

Of \mathbf{k} genotypes, \mathbf{x} is female and \mathbf{y} is male one. At a certain stage, the females of genotype \mathbf{f}_a and males of genotypes \mathbf{m}_a form a pair then descendants appear. The other symbols are explained in the description of the input parameters of the model.

Table 1. A cycle of the model work.

Symbol	Meaning	Transformation	Changing the number of individuals in the groups
${}^a\mathbf{n}^g_a$	The initial numbers of individuals in groups of a certain genotypes and age in each cycle	Start of cycle	${}^a\mathbf{n}^g_a = \omega_{t-1}\mathbf{n}^g_a$
		Transition individuals to the next age	$\beta\mathbf{n}^g_a = \alpha\mathbf{n}^g_{a-1}$
$\beta\mathbf{n}^g_a$	The numbers of individuals in groups with allowance for their transition to the next age	Non-competitive death	$\gamma\mathbf{n}^g_a \approx \beta\mathbf{n}^g_a \times \mathbf{s}^g_a$
$\gamma\mathbf{n}^g_a$	The numbers of individuals in groups after non-competitive mortality		
$\delta\mathbf{n}^g_a$	The numbers of individuals in groups after joining immigrants	Immigration	$\delta\mathbf{n}^g_a = \gamma\mathbf{n}^g_a + \mathbf{i}^g_a$
		Competitive reduction in number of individuals	Algorithm of the calculation $\omega\mathbf{n}^g_a$ based on $\delta\mathbf{n}^g_a$, \mathbf{c}^g_a , \mathbf{d}^g_a and \mathbf{V} (it is described below)
$\omega\mathbf{n}^g_a$	The numbers of individuals in groups after competitive mortality due to lack of resources	Creation of the parental pairs	Algorithm of the calculation $\mathbf{P}(\mathbf{f}_a, \mathbf{m}^m_{a'})$ based on $\omega\mathbf{n}^f_a$, \mathbf{l}^f_a , $\omega\mathbf{n}^m_{a'}$ and $\mathbf{e}^m_{a'}$ (it is described separately below)
$\mathbf{P}(\mathbf{f}_a, \mathbf{m}^m_{a'})$	Number of pairs of a certain composition		
$\omega\mathbf{n}^g_0$	The number of offspring ($\mathbf{a}=0$)	Reproduction	$\omega\mathbf{n}^g_0 = \Sigma(\mathbf{P}(\mathbf{f}_a, \mathbf{m}^m_{a'}) \times \mathbf{o}^g(\mathbf{f}^f, \mathbf{m}^m) \times \mathbf{b}^f_a \times \mathbf{w}^m_{a'})$
		End of cycle	

2.2 Input Parameters

Viability parameters. $s_a^g \in [0,1]$ — *survival*. This is proportion of individuals, which happens to be saved in a result of non-competitive death. If $a \geq \max a_a^g$, then $s_a^g = 0$ where $\max a_a^g$ stands for the maximum life span, and a is the age of individual.

$c_a^g \in [0,1]$ — *competitiveness factor*. Let's designate the probability of an individual to survive over the competitive reduction as c_a^g . Denote $\max c'$ as the maximum value of this probability that is characteristic for representatives of the most competitive groups ($0 < \max c' \leq 1$). According to algorithm of the competitive reduction, the number of the entire HPC along with the value of competitiveness affects a probability to survive for each individual. The value of the competitiveness factor $c_a^g = c_a^g / \max c'$ can be defined as one of the input parameters of the model.

$d_a^g, (d_a^g \geq 0)$ — *demand*. This is the number of resources required for individual of a certain group. It's magnitude is given for one cycle of the model.

$l_a^f \in [0,1]$ — *female loveliness*. This is the female success rate in its search for a partner for reproduction. That is set in the same way as the competitiveness factor is specified. Let's denote the maximum value of the probability to find a partner as $\max l'$, ($0 < \max l' \leq 1$). That is characteristic for the representatives of the most successful groups of females. $l_a^f = l_a^f / \max l'$. Denote the $\text{mat} a_a^g$ as the age of sexual maturity. For females with the age less than $\text{mat} a_a^g$ ($a < \text{mat} a_a^g$), $l_a^f = 0$.

Similarly, $e_a^m \in [0,1]$ — *male effectiveness*. This is the male success rate in its search for a partner for reproduction. Correspondingly, $e_a^m = e_a^m / \max e'$. For males, the age of which ($a < \text{mat} a_a^g$), $e_a^m = 0$.

$b_a^f \in \mathbb{N}$ — *breed*. This is the female fertility. That is specified by the number of eggs produced by the females.

$w_a^m \in [0,1]$ — *wad*. This is ability of the males to fertilize. It is measured by a fraction of eggs that should be fertilized by a given male.

$o^g(f^f, m^m) \in [0,1]$ — *offspring*. This is the proportion of the descendants of the g-th genotype of the female's f-genotype with the male's m-genotype. That is set for all possible genotypes for entire pairs $P(f^f, m^m)$.

Conditions for experiment. The following global settings should be set to run an experiment or series of experiments.

$o n_a^g \in \mathbb{N}$ — *number*, which is the initial number of all groups.

$i_a^g \in \mathbb{N}$ — *inbound*, which is number of individual-immigrants at a certain cycle (t) provided by the experiment script.

V — *volume* — availability of resources that is amount of resources provided by habitat. It is measured in the number of resource units.

2.3 The Algorithm of the Model

A cycle of the model work is described in the Table 1. The table describes variations in the numbers of individual groups. However, in the model, calculations are made for each individual and then summarized for the groups of individuals. For example, for a non-competitive reduction of quantities $\gamma_t n_a^g \approx \beta_t n_a^g \times s_a^g$. This process is implemented

stochastically, and that explains usage of sign \approx , and not $=$. The pseudo-random number generator defines the fate of each individual of the every genotype and every age. An individual survives with probability s_a^g , and dies with probability $1-s_a^g$.

Algorithm of the competitive mortality rate. Denote the ${}^{\delta}\mathbf{D} = \Sigma({}^{\delta}\mathbf{t}\mathbf{n}_a^g \times \mathbf{d}_a^g)$,

${}^{\varepsilon}\mathbf{t}\mathbf{n}_a^g = {}^{\delta}\mathbf{t}\mathbf{n}_a^g \times \mathbf{c}_a^g$ and ${}^{\varepsilon}\mathbf{D} = \Sigma({}^{\varepsilon}\mathbf{t}\mathbf{n}_a^g \times \mathbf{d}_a^g)$.

If ${}^{\delta}\mathbf{D} \leq \mathbf{V}$, then ${}^{\omega}\mathbf{t}\mathbf{n}_a^g = {}^{\delta}\mathbf{t}\mathbf{n}_a^g$.

If ${}^{\delta}\mathbf{D} > \mathbf{V}$ and ${}^{\varepsilon}\mathbf{D} = \mathbf{V}$, then ${}^{\omega}\mathbf{t}\mathbf{n}_a^g \approx {}^{\varepsilon}\mathbf{t}\mathbf{n}_a^g$.

If ${}^{\delta}\mathbf{D} > \mathbf{V}$ and ${}^{\varepsilon}\mathbf{D} > \mathbf{V}$, then ${}^{\omega}\mathbf{t}\mathbf{n}_a^g \approx {}^{\varepsilon}\mathbf{t}\mathbf{n}_a^g \times \mathbf{V} / {}^{\varepsilon}\mathbf{D}$.

If ${}^{\delta}\mathbf{D} > \mathbf{V}$ and ${}^{\varepsilon}\mathbf{D} < \mathbf{V}$, then ${}^{\omega}\mathbf{t}\mathbf{n}_a^g \approx {}^{\delta}\mathbf{t}\mathbf{n}_a^g - ({}^{\delta}\mathbf{t}\mathbf{n}_a^g - {}^{\varepsilon}\mathbf{t}\mathbf{n}_a^g) \times ({}^{\delta}\mathbf{D} - \mathbf{V}) / (\mathbf{V} - {}^{\varepsilon}\mathbf{D})$.

The fate of each individual of each genotype and each age is determined by the pseudo-random number generator. They survive with probability ${}^{\omega}\mathbf{t}\mathbf{n}_a^g / {}^{\delta}\mathbf{t}\mathbf{n}_a^g$ and die with probability $1 - {}^{\omega}\mathbf{t}\mathbf{n}_a^g / {}^{\delta}\mathbf{t}\mathbf{n}_a^g$.

Such a reduction in the quantities satisfies the following conditions:

1) Quantity before reduction is reduced up to the value that corresponds to resource availability.

2) Quantity of each group before the competitive reduction, ${}^{\delta}\mathbf{t}\mathbf{n}_a^g$, is reduced to a quantity after competitive reduction, ${}^{\omega}\mathbf{t}\mathbf{n}_a^g$, in such a way that percent of individuals of each group, which passed through the competitive reduction, is proportional to the competitiveness of this group's representative: ${}^{\omega}\mathbf{t}\mathbf{n}_a^g / {}^{\delta}\mathbf{t}\mathbf{n}_a^g \sim \mathbf{c}_a^g$.

Algorithm of creation of the parental pairs. The quantity of the female's \mathbf{f}_a and the male's \mathbf{m}_a^m pairs is determined in the following way:

$\mathbf{P}(\mathbf{f}_a, \mathbf{m}_a^m) \approx {}^{\omega}\mathbf{n}_a^f \times ({}^{\omega}\mathbf{n}_a^f \times \mathbf{f}_a / \Sigma({}^{\omega}\mathbf{n}_a^f \times \mathbf{f}_a)) \times ({}^{\omega}\mathbf{n}_a^m \times \mathbf{e}_a^m / \Sigma({}^{\omega}\mathbf{n}_a^m \times \mathbf{e}_a^m))$.

The total number of females from the group \mathbf{f}_a is multiplied by the probability for the females of the group to be selected by any male. This allows you to set the number of the females in the group, who should find a partner in this iteration. The resulting number is multiplied by the probability for the male of the group \mathbf{m}_a^m to be chosen by any female. In this way one can identify the females from group \mathbf{f}_a , which form a pair with the male from group \mathbf{m}_a^m .

The probability for the females from the group \mathbf{f}_a to find a partner is determined by the ratio of the product of quantity of this group ${}^{\omega}\mathbf{n}_a^f$ and the success factor of this group of representatives in finding a partner \mathbf{f}_a , to the sum of such products for all groups of females.

The probability for the males from the group \mathbf{m}_a^m to find a female is determined by the ratio of the product of quantity of this group ${}^{\omega}\mathbf{n}_a^m$ and the success factor of this group of representatives in finding a partner \mathbf{e}_a^m to the sum of such products for all groups of males.

The fate of each particular female and male is determined by the random number generator in accordance with the probabilities, given the expected number of pairs of $\mathbf{P}(\mathbf{f}_a, \mathbf{m}_a^m)$.

3 Selection of Parameters

The adequacy of the model was tested on the processes observed in the all-diploid HPS from the Siverskyi Donets center of diversity of the *Pelophylax esculentus* complex. In total, eight different genomes can be transmitted in HPS of these water frogs (Table 2).

In the Siverskyi Donets center of diversity of the *Pelophylax esculentus* complex there are no mature *P. lessonae*, and therefore are no genomes of X^L and Y^L . In this paper, we have considered only diploid frogs. Therefore, in the simulation described only eight genotypes were considered as shown in Table 3.

Table 2. The genomes considered in the model.

Genome	X^L	Y^L	X^R	Y^R	(X^L)	(Y^L)	(X^R)	(Y^R)
Mode of inheritance	Recombinant				Clonal			
Species	<i>P. lessonae</i>		<i>P. ridibundus</i>		<i>P. lessonae</i>		<i>P. ridibundus</i>	
Sex	Female	Male	Female	Male	Female	Male	Female	Male

Table 3. The genotypes considered in this work.

	Females	Males
<i>P. ridibundus</i>	$X^R X^R$	$X^R Y^R$
<i>P. esculentus</i>	$X^R(X^L), (X^L)(X^R)$	$X^R(Y^L), Y^R(X^L), (X^L)(Y^R), (Y^L)(X^R)$.

The set of genomes is defined as $G = [0, 1]^4 \times \{0, 1\}^2 \subset R^4$. An individual is designated by three parameters: age $A \in N$ and two genomes (g1 and g2). Thus, a set of individuals is $A \times G \subset R^{13}$.

The set of HPS systems $HPS = \Phi^{N+M} \subset R^{13(N+M)}$ consists of $N + M$ frogs, where N is the size of the spawning HPS, and M stands for the number of immature individuals.

The following data input is used in the model:

- A description of the initial composition of the model HPS, and the scenario of migrants entering into it;
- A description of the parameters of the viabilities for all considered groups of individuals that differ by age and by genomic composition;
- A description of the results of all possible crossings in the model (distribution of the probability of occurrence of offspring with a specific genomic composition from a crossing of different parents).

A detailed justification of the chosen default settings is beyond the scope of this work. It is done on the basis of study of the natural HPS, including above all the determination of the lifespan and the frog's growth rates using skeletochronology data, and results from the estimation of the population size and composition of the natural HPS by the mark-and-recapture method. Assumptions about the results of crossings (Table 4) were made based on the results of a study of the nature of gametogenesis of hybrid frogs from the Siverskyi Donets center of diversity of the *Pelophylax esculentus* complex [2]. The model assumes that resource consumption is proportional to the biomass of the individual. Empty cells in the Table 4 correspond to the crossings of which the offspring are non-viable. In cases when a cell, corresponding to a certain crossing, contains 2, 3 or 4 genotype, the descendants that correspond to these genotypes appear with equal probability (corresponding to $\frac{1}{2}$, $\frac{1}{3}$, or $\frac{1}{4}$).

A preliminary research was carried out to determine the age structure of the model HPS in which we determined the equilibrium age structure of the HPS *P. ridibundus*. In further experiments, the age distribution of the initial composition of HPS corresponds to that age structure. In those cases when we added the new specimens into HPS at a certain step, they were considered as 4 years old.

Table 4. The proposed crossing results, assumed at modelling.

Genotypes	♂♂	$x_R y_R$		$x_R(y_L)$	$y_R(x_L)$	$(x_L)(y_R)$		$(y_L)(x_R)$	
♀♀	Gametes	x_R	y_R	(y_L)	(x_L)	(x_L)	(y_R)	(y_L)	(x_R)
$x_R x_R$	x_R	$x_R x_R$	$x_R y_R$	$x_R(y_L)$	$x_R(x_L)$	$x_R(x_L)$	$x_R y_R$	$x_R(y_L)$	$x_R x_R$
$x_R(x_L)$	(x_L)	$x_R(x_L)$	$y_R(x_L)$	—	—	—	$(x_L)(y_R)$	—	$(x_L)(x_R)$
$(x_L)(x_R)$	(x_L)	$x_R(x_L)$	$y_R(x_L)$	—	—	—	$(x_L)(y_R)$	—	$(x_L)(x_R)$
	(x_R)	$x_R x_R$	$x_R y_R$	$(y_L)(x_R)$	$(x_L)(x_R)$	$(x_L)(x_R)$	$x_R y_R$	$(y_L)(x_R)$	$x_R x_R$

4 Case Studies

4.1 The Space of Possible Outcomes of the HPS Transformations

To determine the set of possible end states of the water frogs' HPS, consisting of diploid representatives, we chose a set of initial states, evenly distributed in the space of possible states. For 8-examined genotypes, the part of each ($p_{\text{♀}}^{x_R x_R}$, $p_{\text{♂}}^{x_R y_R}$ etc.) varied in increments of $\frac{1}{8}$ from 0 to $\frac{7}{8}$. Total $8! = 16,777,216$ such combinations are possible. Of this amount, the combinations that satisfy the following conditions were selected:

$$\begin{aligned}
& p_{\text{♀}}^{\text{X}}\text{R}^{\text{X}}\text{R} + p_{\text{♂}}^{\text{X}}\text{R}^{\text{Y}}\text{R} + p_{\text{♀}}^{\text{X}}\text{R}^{\text{X}}\text{L} + p_{\text{♂}}^{\text{X}}\text{R}^{\text{Y}}\text{L} + p_{\text{♂}}^{\text{Y}}\text{R}^{\text{X}}\text{L} + p_{\text{♀}}^{\text{X}}\text{L}^{\text{X}}\text{R} + \\
& p_{\text{♂}}^{\text{X}}\text{L}^{\text{Y}}\text{R} + p_{\text{♂}}^{\text{Y}}\text{L}^{\text{X}}\text{R} = 1; \\
& p_{\text{♀}}^{\text{X}}\text{R}^{\text{X}}\text{R} + p_{\text{♀}}^{\text{X}}\text{R}^{\text{X}}\text{L} + p_{\text{♀}}^{\text{X}}\text{L}^{\text{X}}\text{R} > 0; \\
& p_{\text{♂}}^{\text{X}}\text{R}^{\text{Y}}\text{R} + p_{\text{♂}}^{\text{X}}\text{R}^{\text{Y}}\text{L} + p_{\text{♂}}^{\text{Y}}\text{R}^{\text{X}}\text{L} + p_{\text{♂}}^{\text{X}}\text{L}^{\text{Y}}\text{R} + p_{\text{♂}}^{\text{Y}}\text{L}^{\text{X}}\text{R} > 0.
\end{aligned}$$

Naturally, it does not make sense to consider the combinations in which the total proportion of genotypes involving into the HPS is not equal to unity, as well as those in which there are no male or female. The total number of genotypes that satisfy the above conditions equals 5895. Ten simulations of 500 steps were conducted for the 5895 starting points. The collection of all observed outcomes of the simulation was divided into types, depending on what kind of genotypes presented in the model HPS over 500 steps. For 4778 initial states, all 10 iterations led to any one outcome. In 1117 cases, outcomes were variable. For these 1117 initial states, 10 more runs were carried out; thus, the total number of simulations was 70,120.

To determine the states, which the model HPS can move to, we examined the intervals between step 100 and 200, step 200 and 300, 300 and 400 as well as 400 and 500. The total number of intervals were 162,580; its number is less than possible one due to the model HPS, which dies at any stage of the simulation.

To divide the obtained set of 70,120 final states of individual simulations into groups, we used the analysis of this aggregation by the method of principal components. The first and the second major components make it possible to divide the HPS into 6 groups (Fig. 3. A):

- Extinction — 37,946 runs ended in HPS extinction;
- R-E-HPS — 22,204 runs ended in different HPSs R-E-types;
- E-HPS-type I — 5884 results; such HPS include $\text{♀}^{\text{X}}\text{L}^{\text{X}}\text{R}$ and $\text{♂}^{\text{X}}\text{L}^{\text{Y}}\text{R}$;
- E-HPS-type II — 3892 results corresponding to another possible type of the E-HPS, which include $\text{♀}^{\text{X}}\text{L}^{\text{X}}\text{R}$ and $\text{♂}^{\text{Y}}\text{L}^{\text{X}}\text{R}$;
- Extincting — 124 results located nearby of the point Extinction. They continue to end up in extinction. The structure of these finals can be further divided into 13 types;
- R-population — 70 results, consisting only of the population *P. ridibundus*.

The R-E-HPS group, which corresponds to 22,204 results by its composition, can be divided into three parts. Their relative positions can be seen in the plane of the first and the third main component (Fig. 3. B):

- Stable R-E-HPS-type I — 18,852;
- Stable R-E-HPS-type II — 2,847 results;
- Indifferent R-E-HPS — 505 results in which *P. ridibundus* is present as well as *P. esculentus*, which transmits both genome *P. lessonae* and female genome *P. ridibundus*.

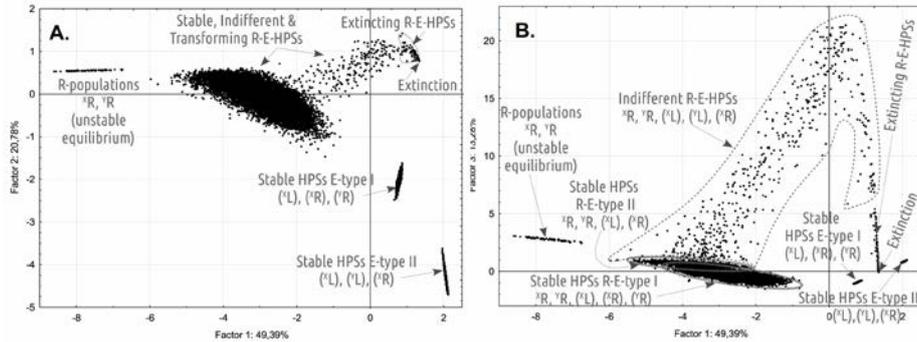


Fig. 3. Ordination of the results of 70,120 simulations. **A.** Ordination of the results on the plane of the first two principal components. **B.** Ordination of the results on the plane of the first and third principal components.

To determine the types of stability for the dynamic types of the allocated HPS, the 162 580 pairs of initial state and its outcome were analyzed. The observed states were classified by the types of stability as shown in Fig. 4.

The observed states are divided into three groups (Equilibrium states, Transient states and Attractive states) as shown in Fig.6, though this division is rather subjective. The Indifferent equilibrium (II) can be considered as a transient state as well. Two versions of the transient states are associated with the directed transitions to other states. Extincting state (IV) is associated with the transition to the extinction state (VI), and transforming stage (III) with the transition to other states.

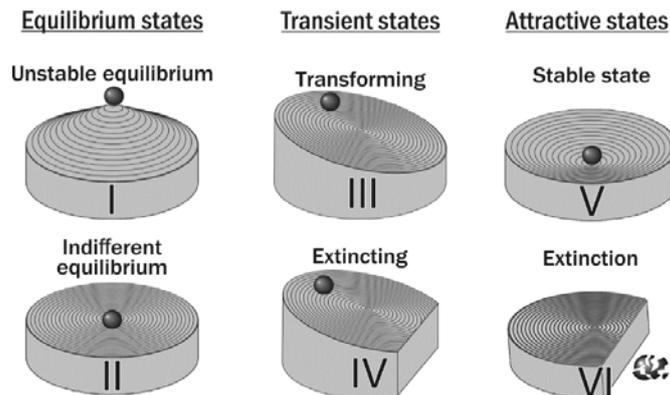


Fig. 4. Types of biosystems stability, observed in experiments with the simulation model.

Six basins of sustainability exist in the space of possible states of HPS that consists of diploid individuals, and this corresponds to specific features of the Sivskyi Donets center of diversity of the *Pelophylax esculentus* complex by their character of the genome transmission. One of them complies with the population of parental species. Two are E-HPS, i.e. spawning population of HPS consisting exclusively of *P. esculentus*. When crossing *P. esculentus* with the hybrid amphispermy, the offspring of parental species appearing in such systems dies before the age of maturity.

E-HPS-type I:

$$\varnothing^{(X_L)(X_R)} \times \varnothing^{(Y_L)(Y_R)} \rightarrow X_L X_L : (X_L)(X_R) : (X_L)(Y_R) : X_R Y_R \rightarrow \varnothing^{(X_L)(X_R)} : \varnothing^{(Y_L)(Y_R)}$$

E-HPS-type II:

$$\varnothing^{(X_L)(X_R)} \times \varnothing^{(Y_L)(X_R)} \rightarrow X_L Y_L : (X_L)(X_R) : (Y_L)(X_R) : X_R X_R \rightarrow \varnothing^{(X_L)(X_R)} : \varnothing^{(Y_L)(X_R)}$$

There are two more basins of stability corresponding to the R-E-HPS containing *P. ridibundus* and *P. esculentus*, and the last basin is associated with extinction of the HPS.

5 Outcome Interpretation

When assessing the results, one must be aware that the result of the simulation is not proof of a hypothesis. At the same time, using simulation models as an exploratory tool has a significant advantage over unformulated conceptual models. We do not have the sufficient empirical data to describe precisely the processes occurring in the natural HPS. The lack of empirical data is offset by a set of presumptions [13] and hypotheses. Simulation allows us to derive consequences arising from the set of initial assumptions.

These sets of consequences may or may not contradict the observable empirical picture. An observed contradiction is the basis for rejecting a set of initial assumptions or adjustments. Agreement is not an evidence for the initial assumptions, but can be seen as an argument in their favor, in other words as corroboration, not as proof (Fig. 5).

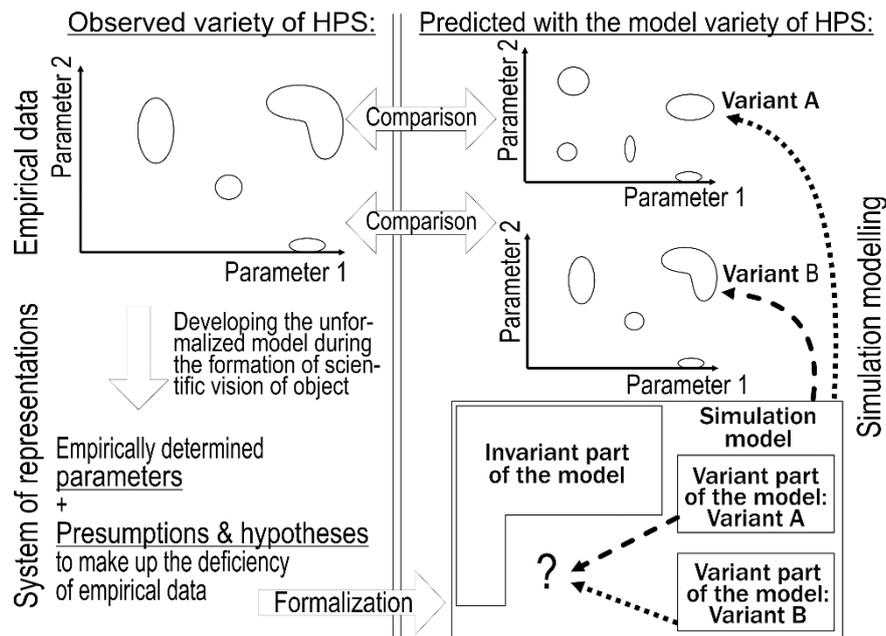


Fig. 5. Using a simulation model to test hypotheses about the mechanisms of HPS functioning. The distribution of the outcomes of the model HPS agrees with the empirical data, and it is obtained in the case when variant B of the variable part of the model is selected. It does not prove variant B to be true, but it allows to discard variant A in its favor.

Fig 5 shows how the simulation results can be used to select between different versions of the assumptions in the absence of empirical data. Model predictions regarding the expected diversity of HPS conditions, depends on assumptions, on which the variant part of the model was constructed. The predicted (modeled) expected diversity of HPS states can be compared to empirically observed diversity of HPS states. The results of this comparison can be seen as the arguments in favor of such initial assumptions that yielded close to the empirical distribution of states HPS.

Simulation results, among other things, stimulate the collection of the empirical data. Comparison of predictions, obtained by modelling, and the available fragmented data about the composition of the natural HPS and character of *P. esculentus* gametogenesis shows that currently there is an absence of E-type HPS in the studied region, although that there are grounds for thinking that such a system probably existed in 1995 [6]. Studying the composition of tadpoles in this pond shows that there existed E-HPS-type II [8]. In fact, the majority of observed systems are in a transient state.

The authors believe that this research is only a starting step in design of the dynamic typology of the water frogs' HPS. The usefulness of the simulation is not limited to fact that two stable states, previously not known to the authors, can theoretically be found: R-E-HPS-type II and E-HPS-type II. Results of simulations allow developing a program for further research. The simulation results define the data collection program for testing the adequacy of the results. The currently available data do not contradict the model findings. Future work will include the study of unstable states of HPS that are observed in the natural environment [16], as well as the extension of the model by incorporating hybrids with three genomes, which are specific for the Siverskyi Donets center of diversity of the *Pelophylax esculentus* complex.

6 Discussion and Conclusion

We study the unusual category of biosystems, Hemiclonal Population Systems (HPS), through the example of the hybridogenic complex of water frogs, the *Pelophylax esculentus* complex. The unusual method of reproduction of interspecific hybrids within HPS results in their unusual features, which need more investigation. An important method for studying such systems is computer simulation.

A simulation model of the water frogs' HPS has been presented. The model inputs are the parameters describing the comparative vitality of various genetic forms of frogs, the results of their probable crossings, as well as the experimental conditions such as the capacity of the environment, the initial composition of the model HPS, and a scenario for the introduction of migrated frogs into the model HPS. Evaluation of the comparative vitality and the crossing results are defined in accordance with the results of population-environmental research in the Siverskyi Donets center of diversity of the *Pelophylax esculentus* complex. Since direct empirical data was lacking, the values of the parameters used have been estimations that authors put forward on the basis of a study of this region.

Repeated runs of the model yield a probability distribution of outcomes of various HPS transformations according to their initial states and experimenter-determined parameters. We analyzed the processes in all-diploid HPS from the Siverskyi Donets center of diversity of the *Pelophylax esculentus* complex, which is characteristic for the Mzha and the Uda river basins. When sampling evenly among the starting point of runs in the space of possible states of such systems, a set of outcomes has been established. Only six stable states have been found for such systems, one of which corresponds to the population of the parental species, two coincide with the HPS consisting of representatives of the parental species and hybrids, two correspond to the HPS consisting solely of hybrid individuals, and one state corresponds to the extinction of frogs in the simulated habitat.

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