DESCRETE MODELS FOR MOLECULAR EVOLUTION: SIMULATION AT THE POPULATION LEVEL

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MOTIVATION:

- Making the process of simulation of ecological or evolutionary process better understandable for a biologist
- Obtaining the results of a simulation in a form which would correspond directly to the outcome of an experiment

Logistic growth with competition and mutations – adaptive dynamics

$$\frac{dN(x,t)}{dt} = r \cdot N(x,t) \cdot \left[1 - \int C_x(x-\chi) N(\chi,t) dy \Big/ K(x)\right]$$

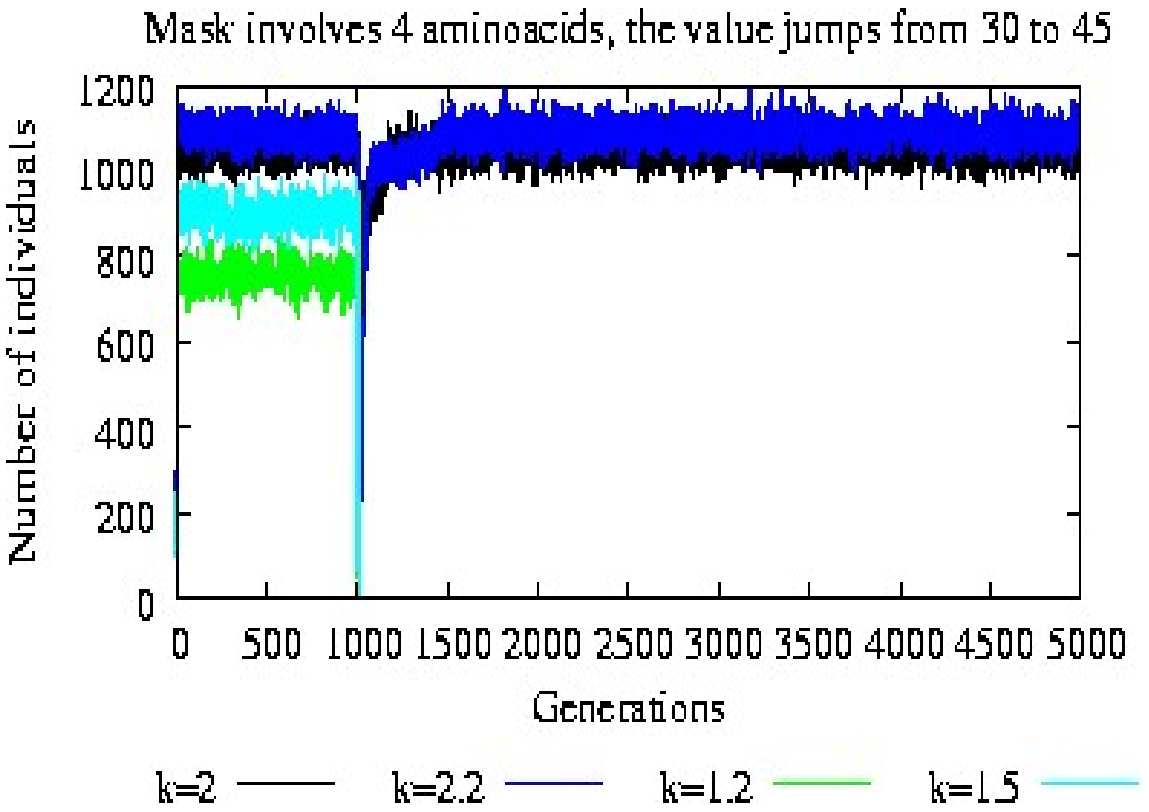
Here x – ecological character defined by polygene

$$K(x) = K_0 \exp\left[-\frac{(x-x_0)^2}{2\sigma_K^2}\right], C_x(z) = \exp\left[-\frac{z^2}{2\sigma_x^2}\right]$$

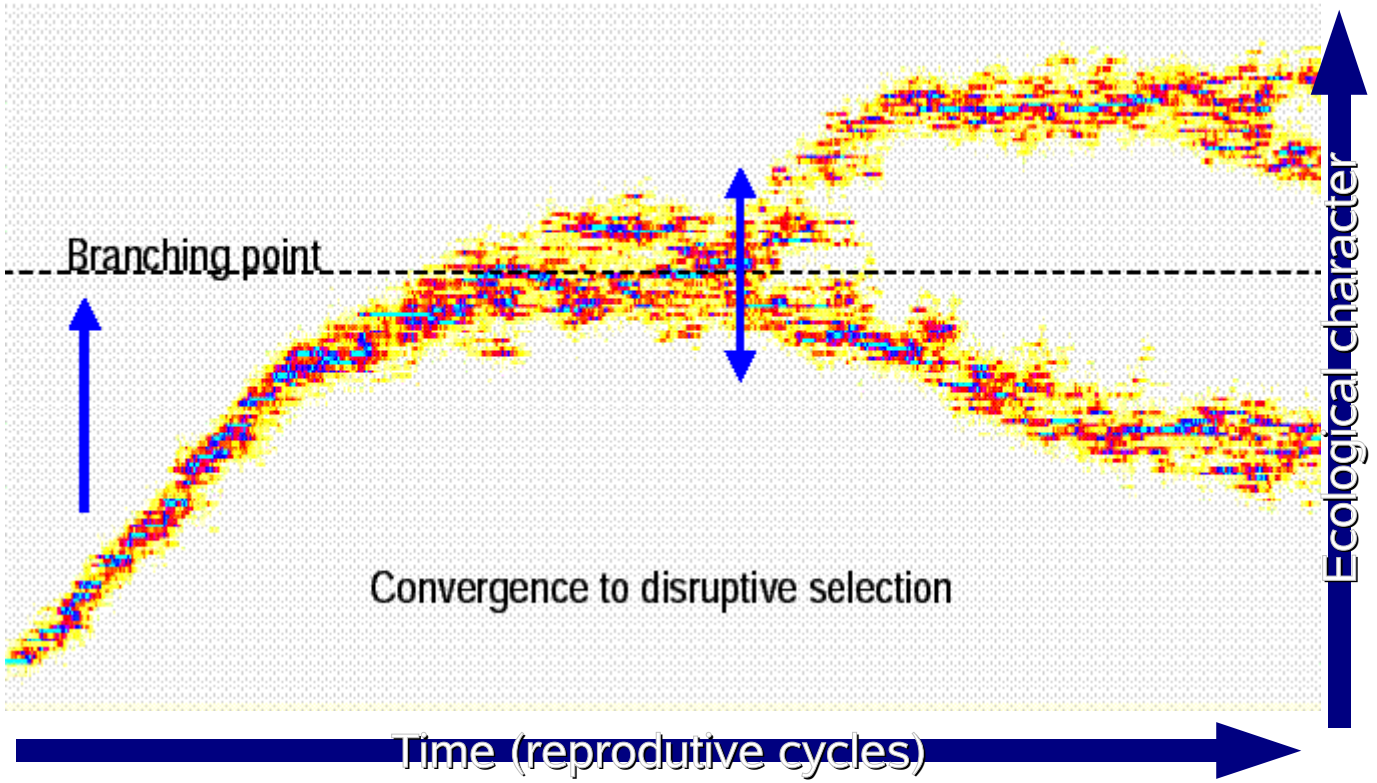
From: On the origin of species by sympatric speciation

Ulf Dieckmann & Michael Doebeli, Nature, 1999

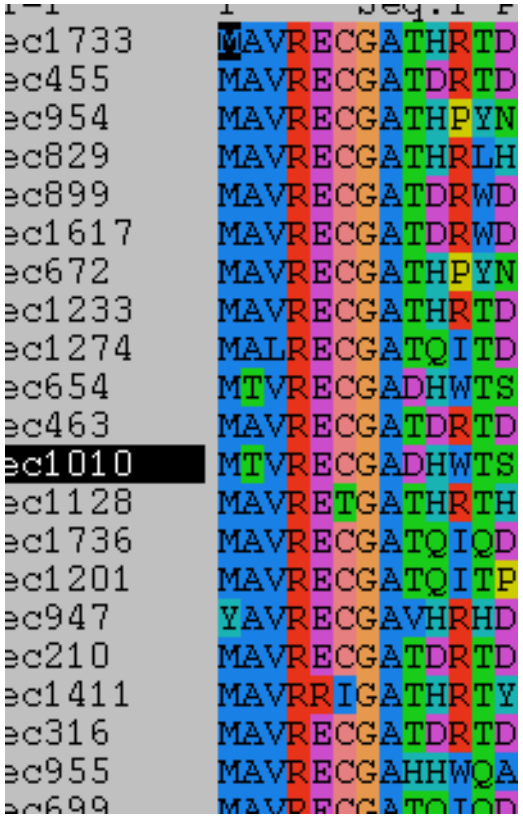
«Useless» simulation

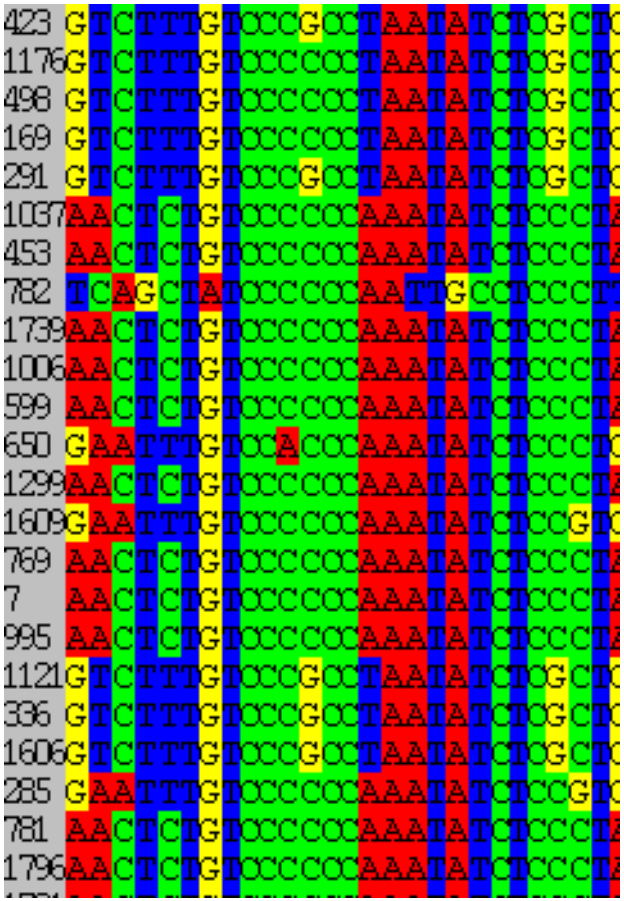


Individual-based representation



Useful simulation, the result is in comfortable format



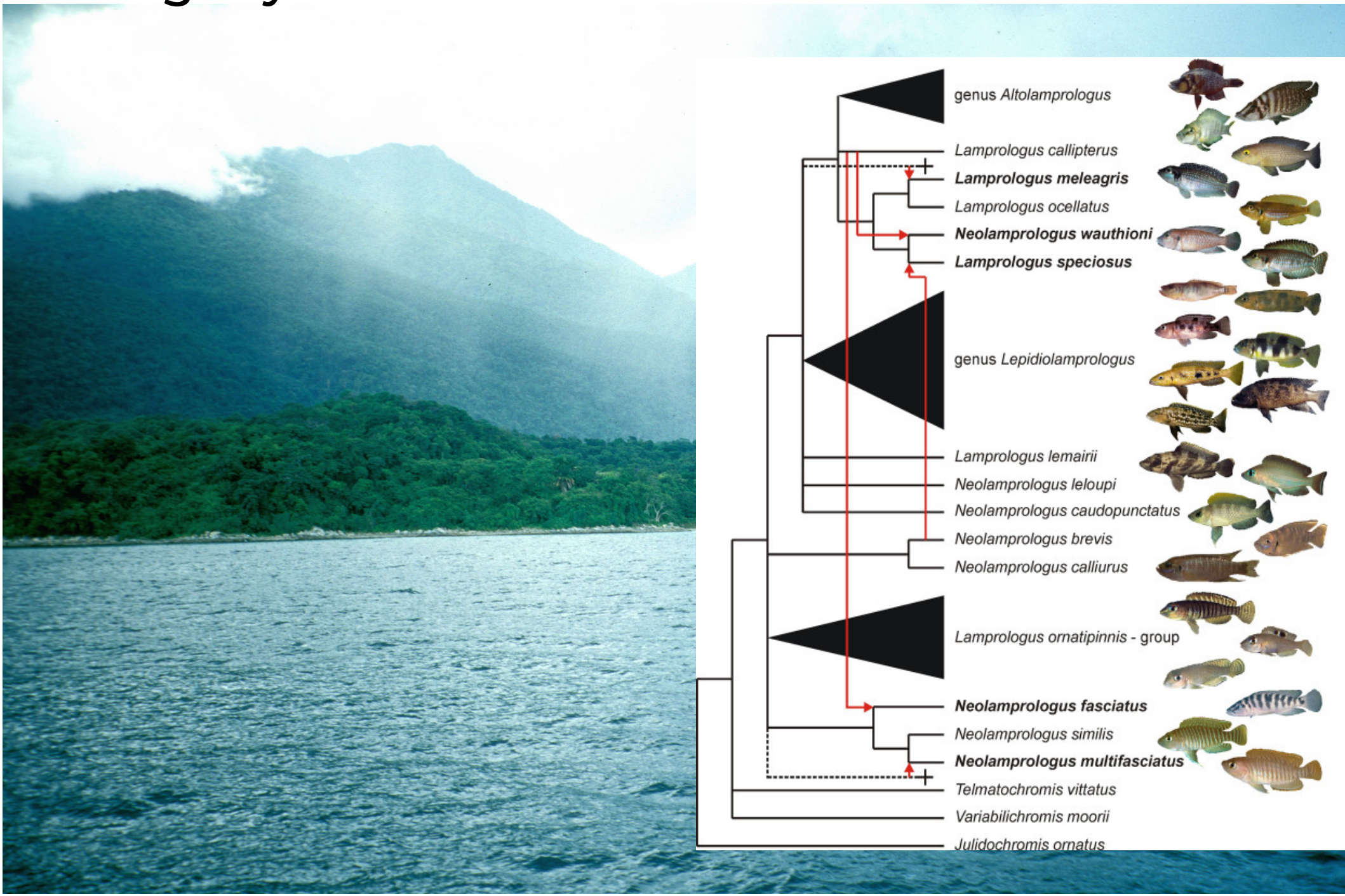


Motivation:
explaining evolution of species flocks

Species flock is a group of species which evolved in confines of the same eco-system from a single ancestor

Species flocks are peculiar to ancient giant freshwater lakes like lake Baikal and Lake Tanganyika, where the most famous and species-rich is set of flocks of ciclids

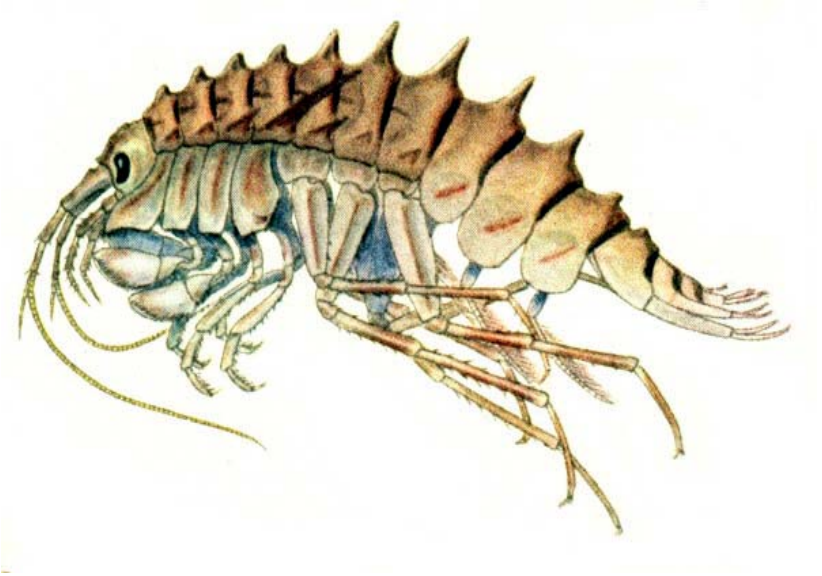
Tanganyika

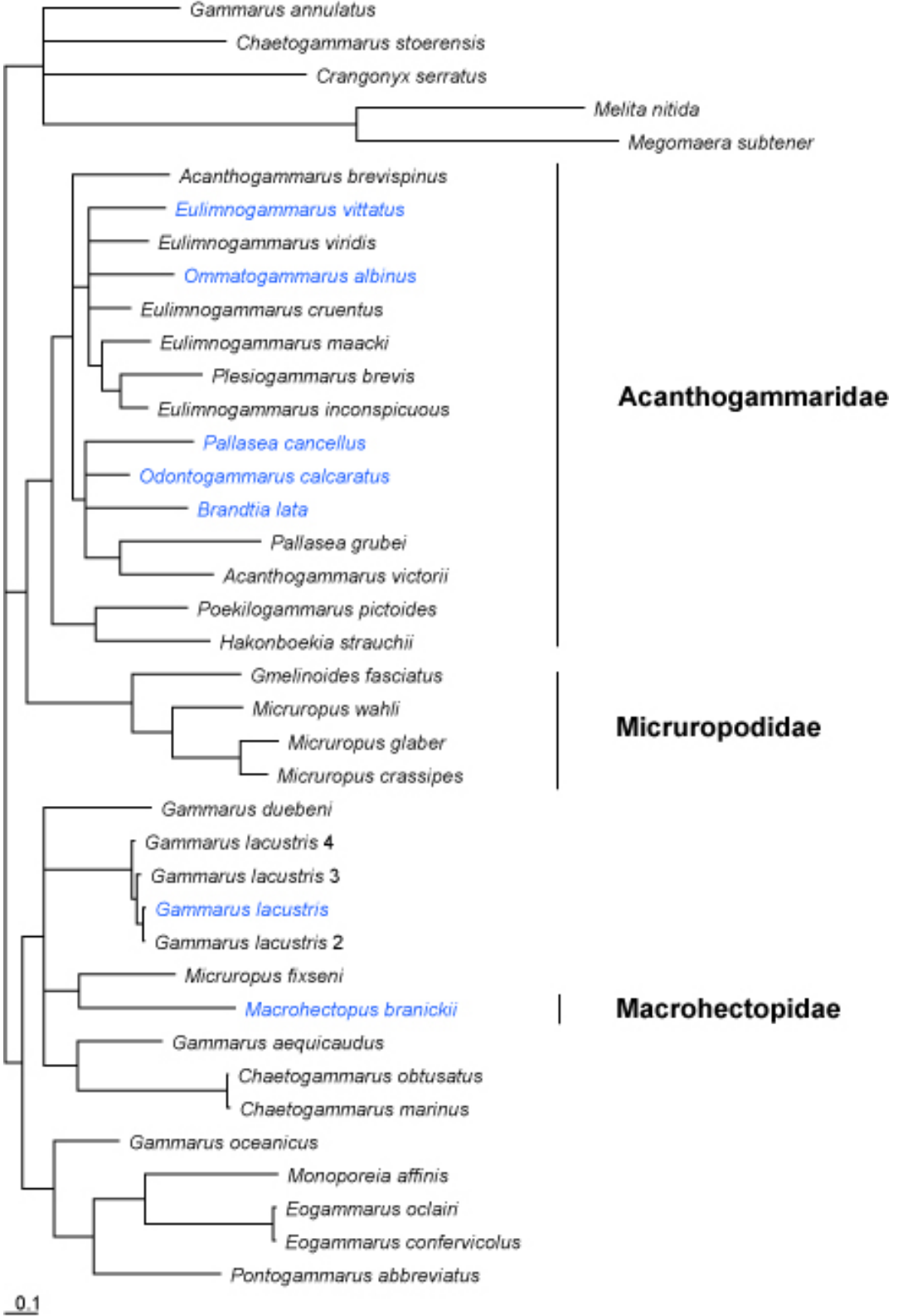

genus Altolamprologus
Lamprologus callipterus
Lamprologus meleagris
Lamprologus ocellatus
Neolamprologus wauthioni
Lamprologus speciosus
genus Lepidiolamprologus
Lamprologus lemairii
Neolamprologus leloupi
Neolamprologus caudopunctatus
Neolamprologus brevis
Neolamprologus calliurus
Lamprologus ornatipinnis - group
Neolamprologus fasciatus
Neolamprologus similis
Neolamprologus multifasciatus
Telmatochromis vittatus
Variabilichromis moorii
Julidochromis ornatus

Tanganyika

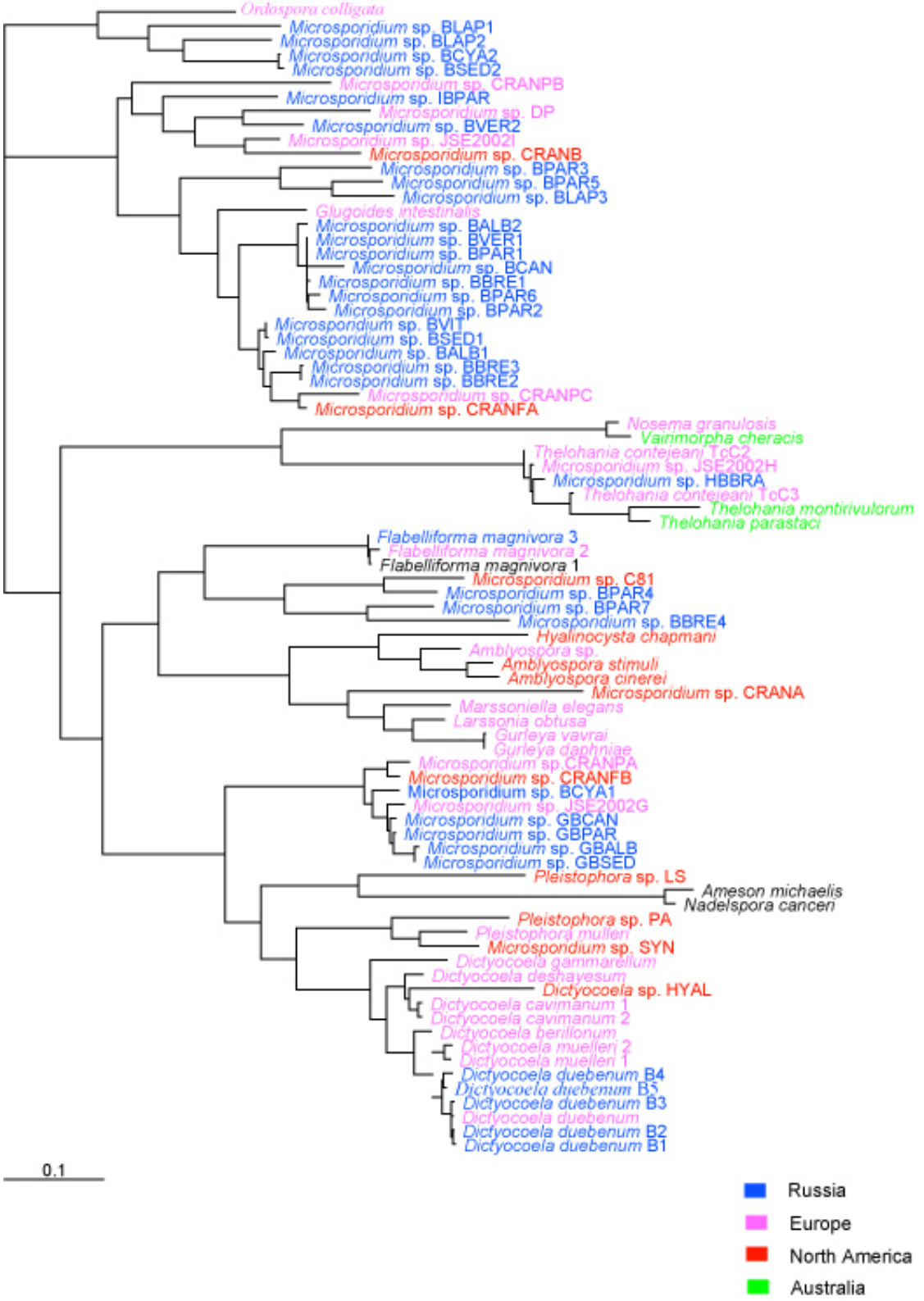

Baikal

Amphipods:




Gammarus annulatus
Chaetogammarus stoerensis
Crangonyx serratus
Melita nitida
Megomaera subtener
Acanthogammarus brevispinus
Eulimnogammarus vittatus
Eulimnogammarus viridis
Ommatogammarus albinus
Eulimnogammarus cruentus
Eulimnogammarus maacki
Plesiogammarus brevis
Eulimnogammarus inconspicuous
Pallasea cancellus
Odontogammarus calcaratus
Brandtia lata
Pallasea grubei
Acanthogammarus victorii
Poekilogammarus pictoides
Hakonboekia strauchii
Acanthogammaridae
Gmelinoides fasciatus
Micruropus wahli
Micruropus glaber
Micruropus crassipes
Micruropodidae
Gammarus duebeni
Gammarus lacustris 4
Gammarus lacustris 3
Gammarus lacustris
Gammarus lacustris 2
Micruropus fixseni
Macrohectopus branickii
Macrohectopidae
Gammarus aequicaudus
Chaetogammarus obtusatus
Chaetogammarus marinus
Gammarus oceanicus
Monoporeia affinis
Eogammarus oclairi
Eogammarus confervicolus
Pontogammarus abbreviatus
0.1

Microsporidia parasiting on Baikalian amphipods comprise the first fully parasitic species flocks. The main surprise here is absolute lack of evidence for any co-evolution between host and parasite. Another problem is co-existence of several parasite species on a single host species: this must cause ultimate extinction of the latter

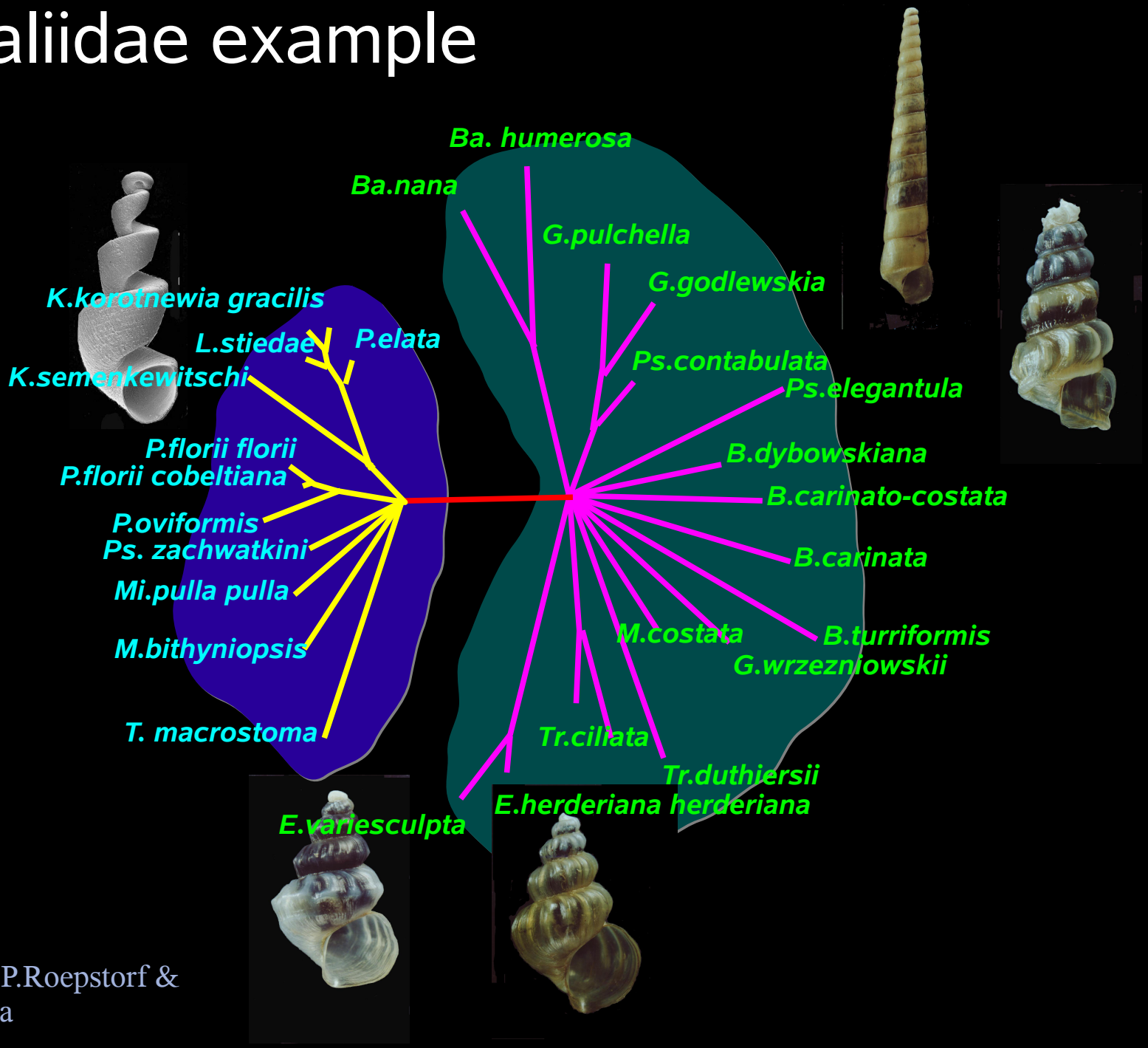


Baicalia carinata

B. dybowskiana

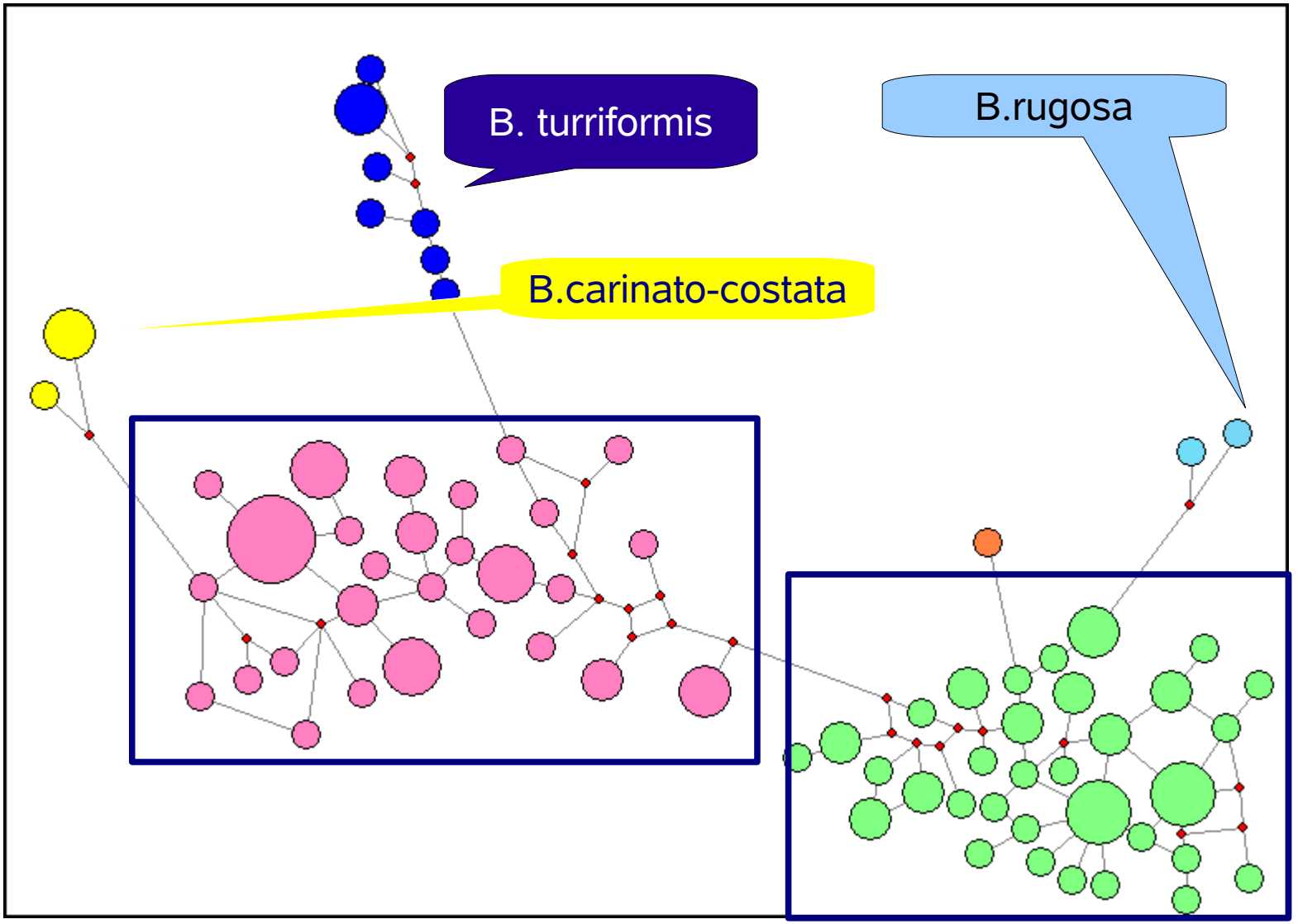
B. turriformis

Baicaliidae example

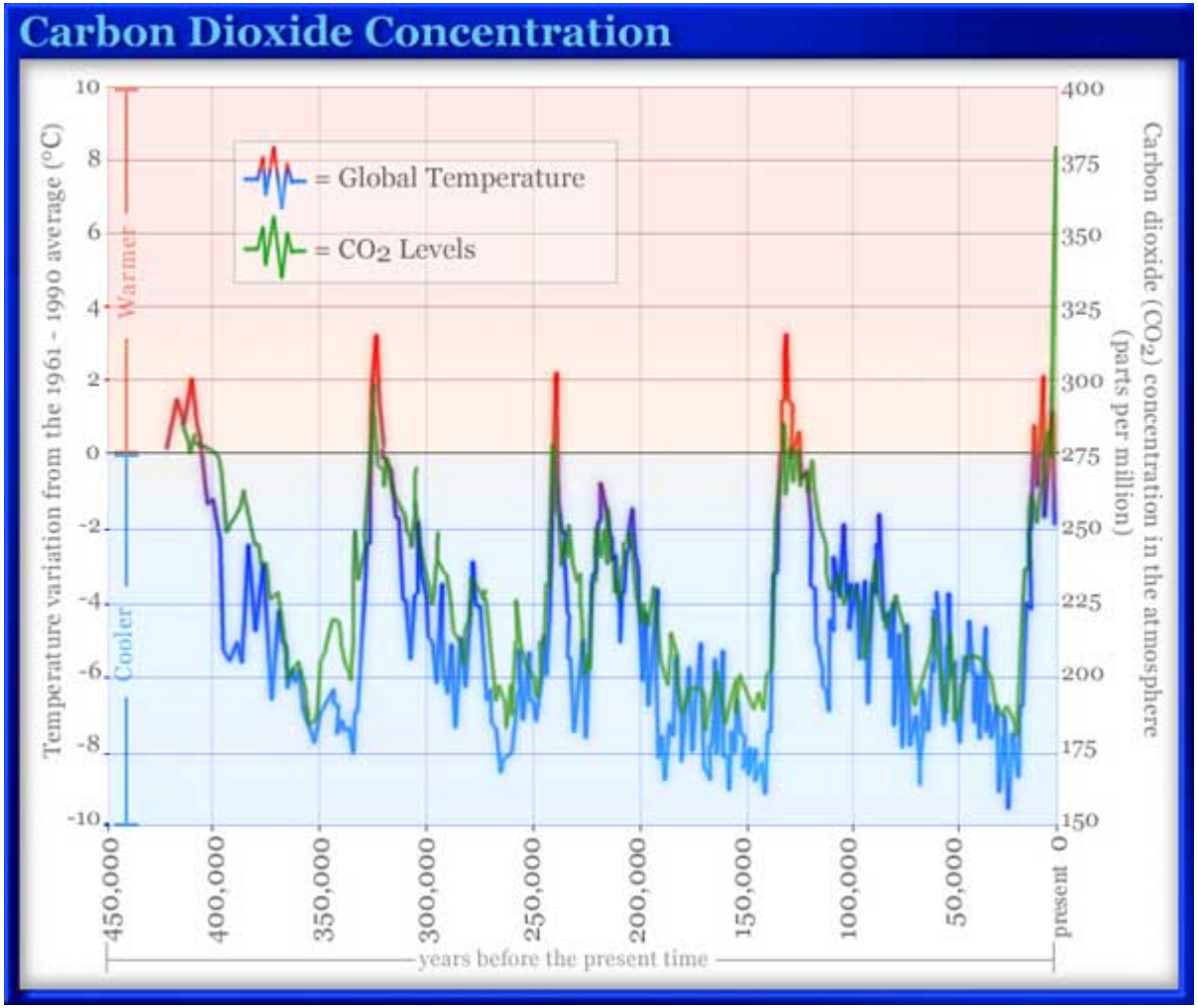


Photos by P.Roepstorf & T.Sitnikova

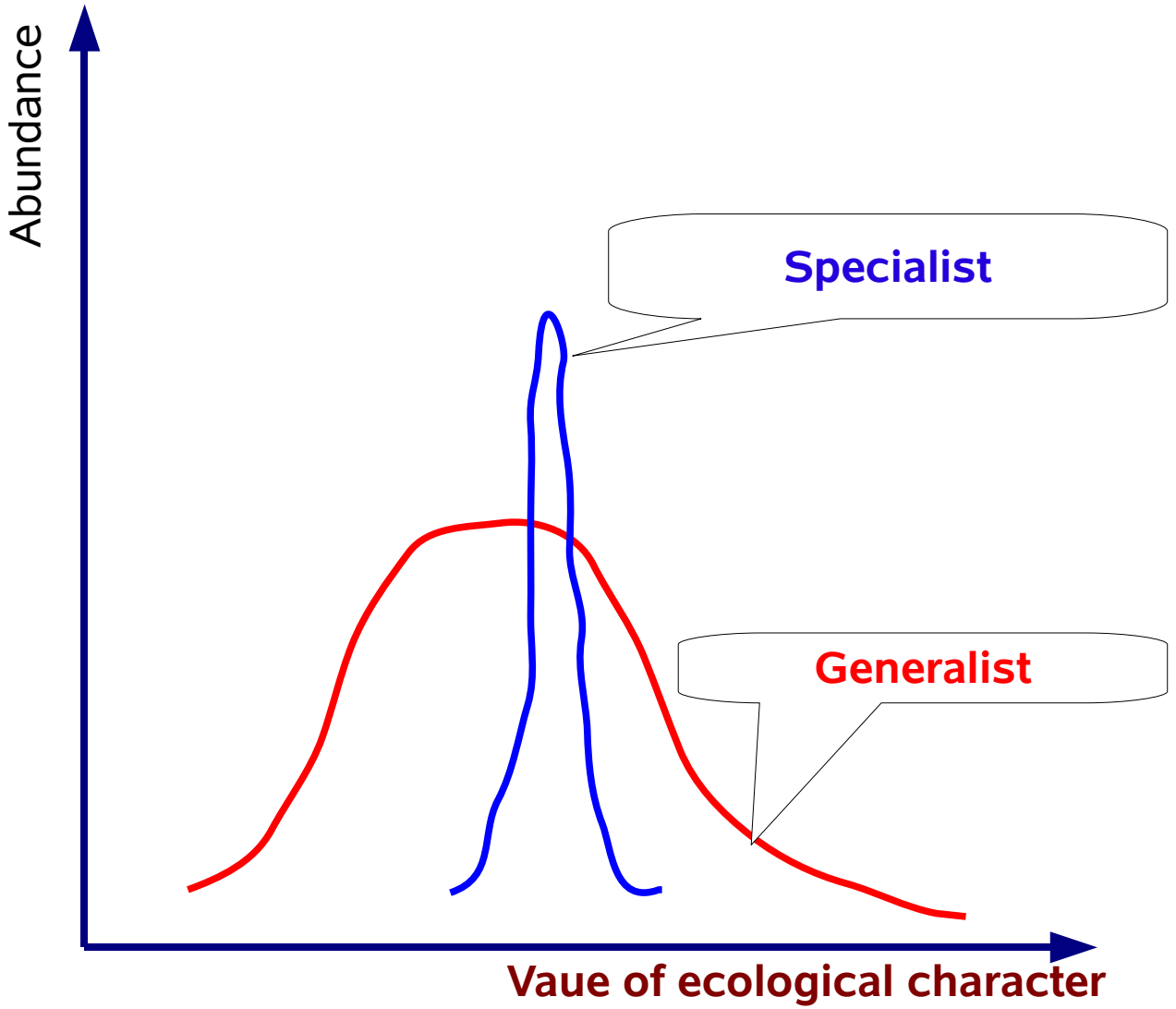
Some evolutionary relations within a flock cannot be represented correctly by a tree



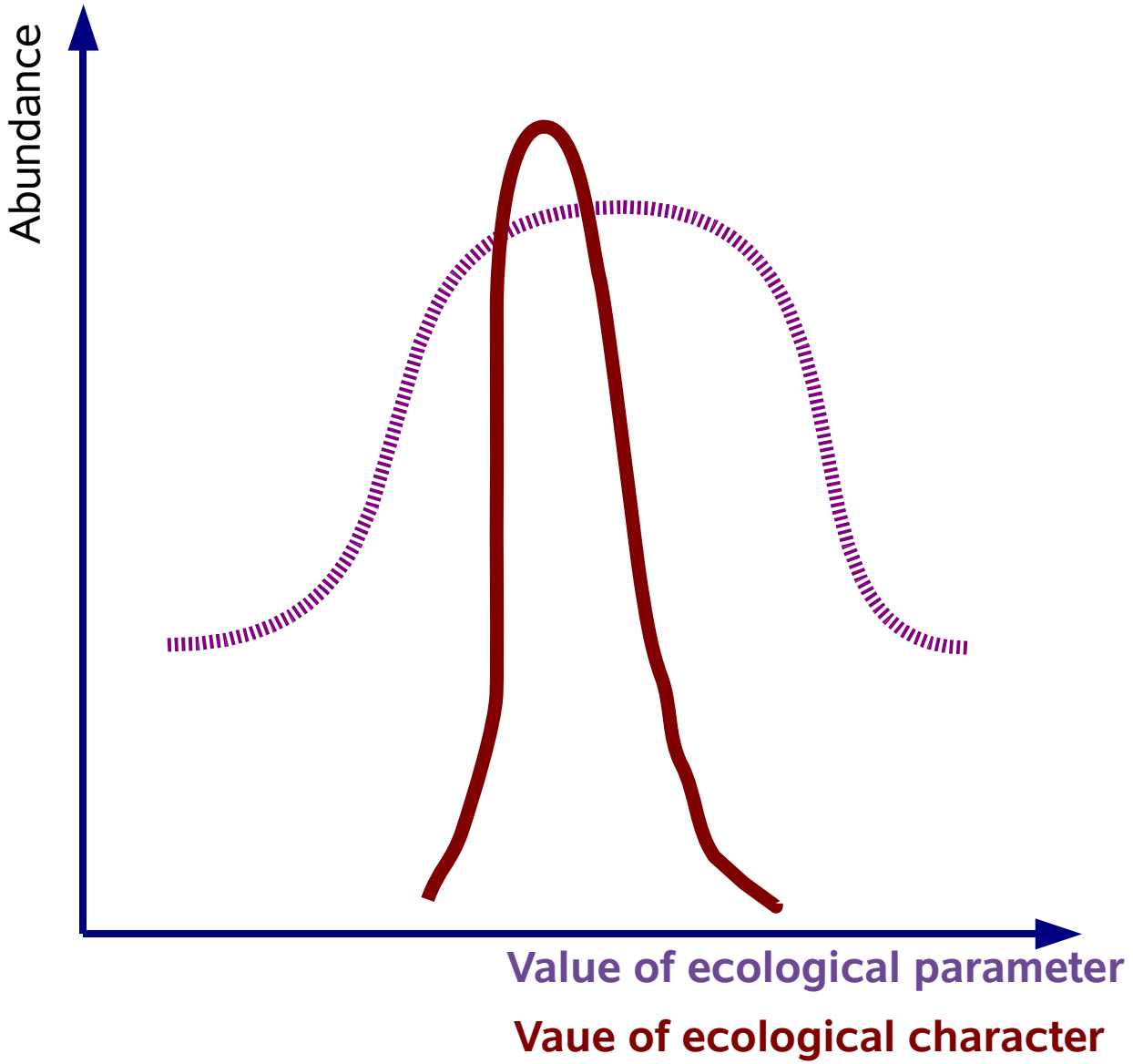
Shackleton cycles: evolution in changing environment



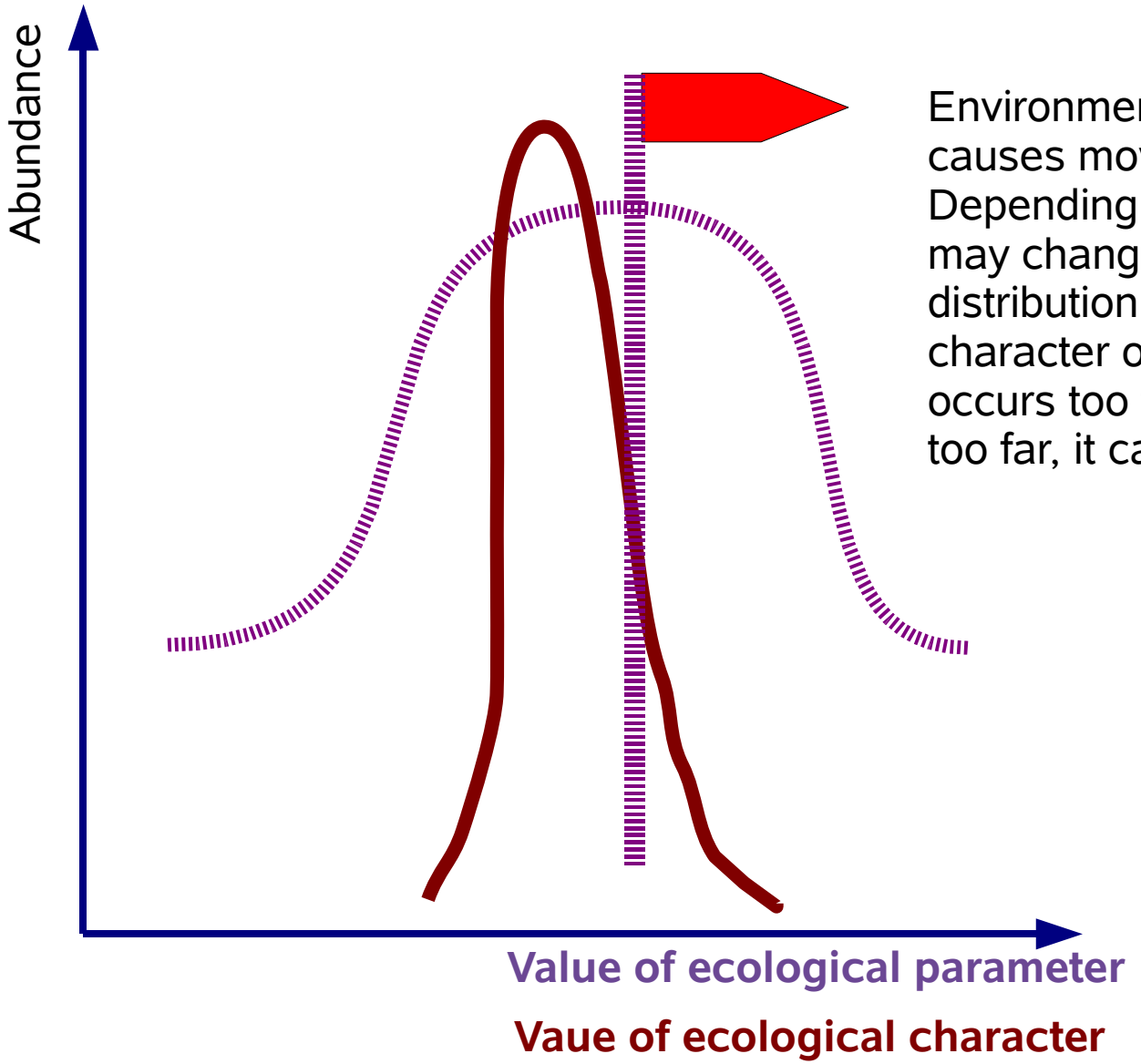
Specialists vs. generalists



Specialists vs. generalists

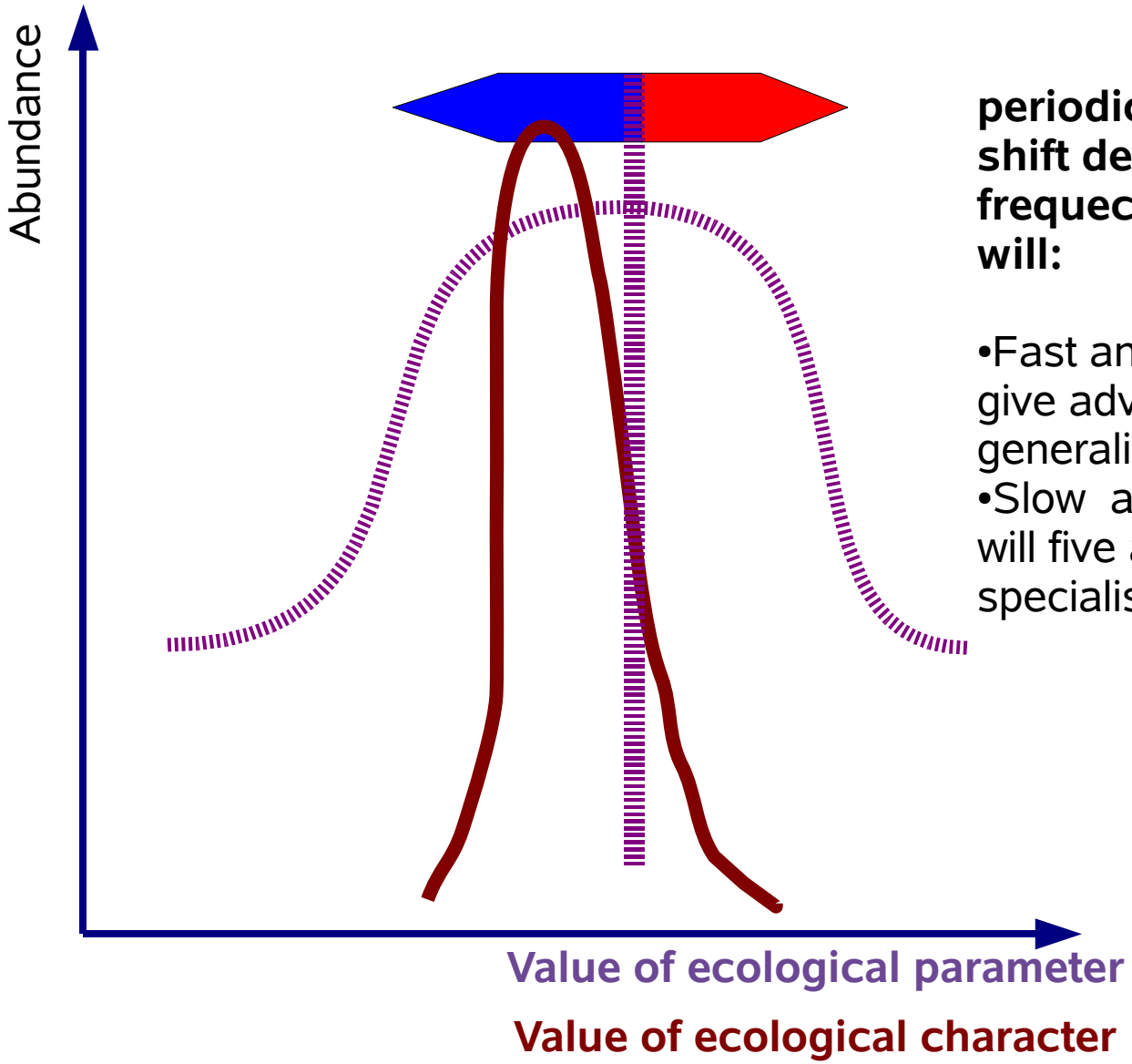


Specialists vs. generalists



Environmental shift causes moving selection. Depending on the speed,it may change the distribution of ecological character of a species. If it occurs too fast and goes too far, it causes extinction

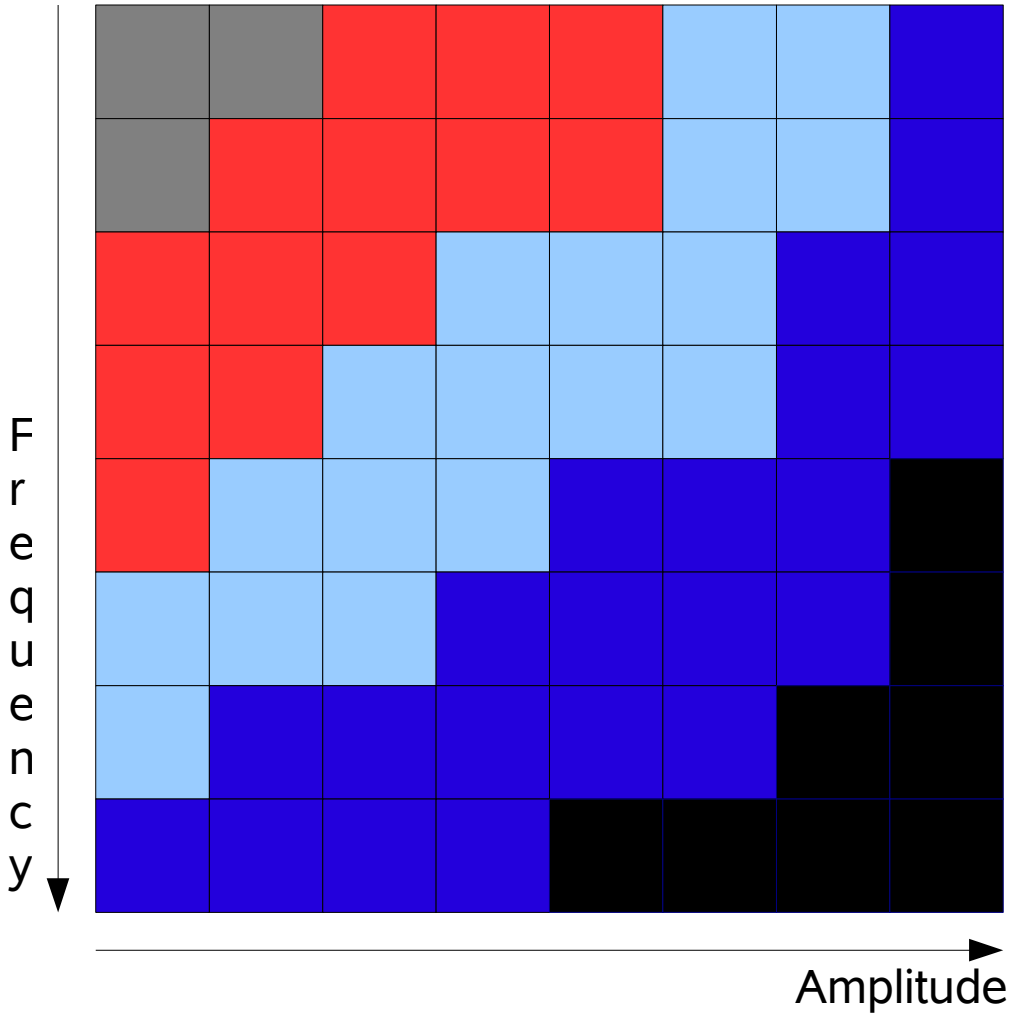
Specialists vs. generalists



periodical environmental shift dependiing on frequecy and amplitude will:

•Fast and wide sweeps will give advantage to generalists;
•Slow and moderate sweeps will five advantage to specialists (narrow niche)

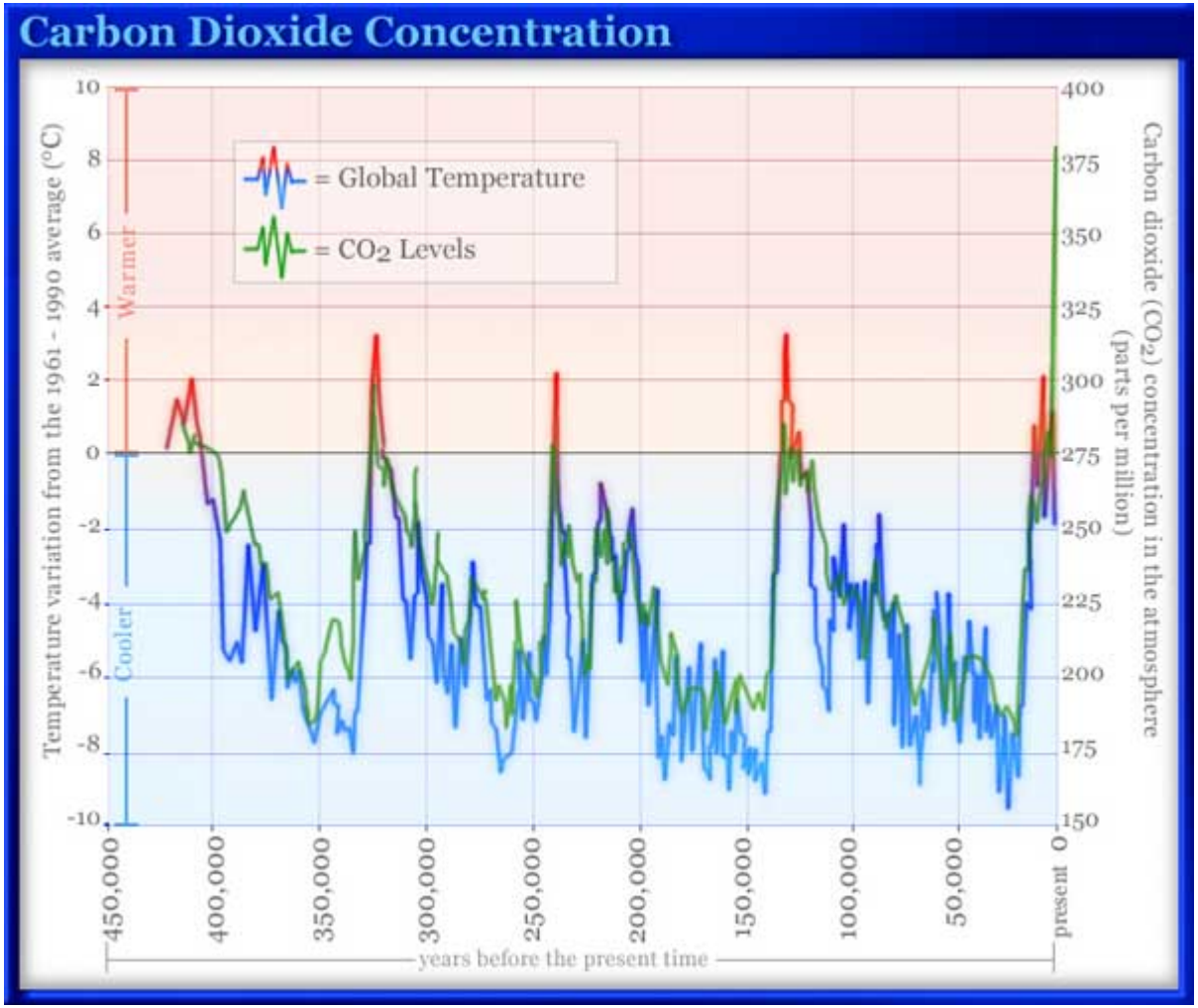
Specialists vs generalists



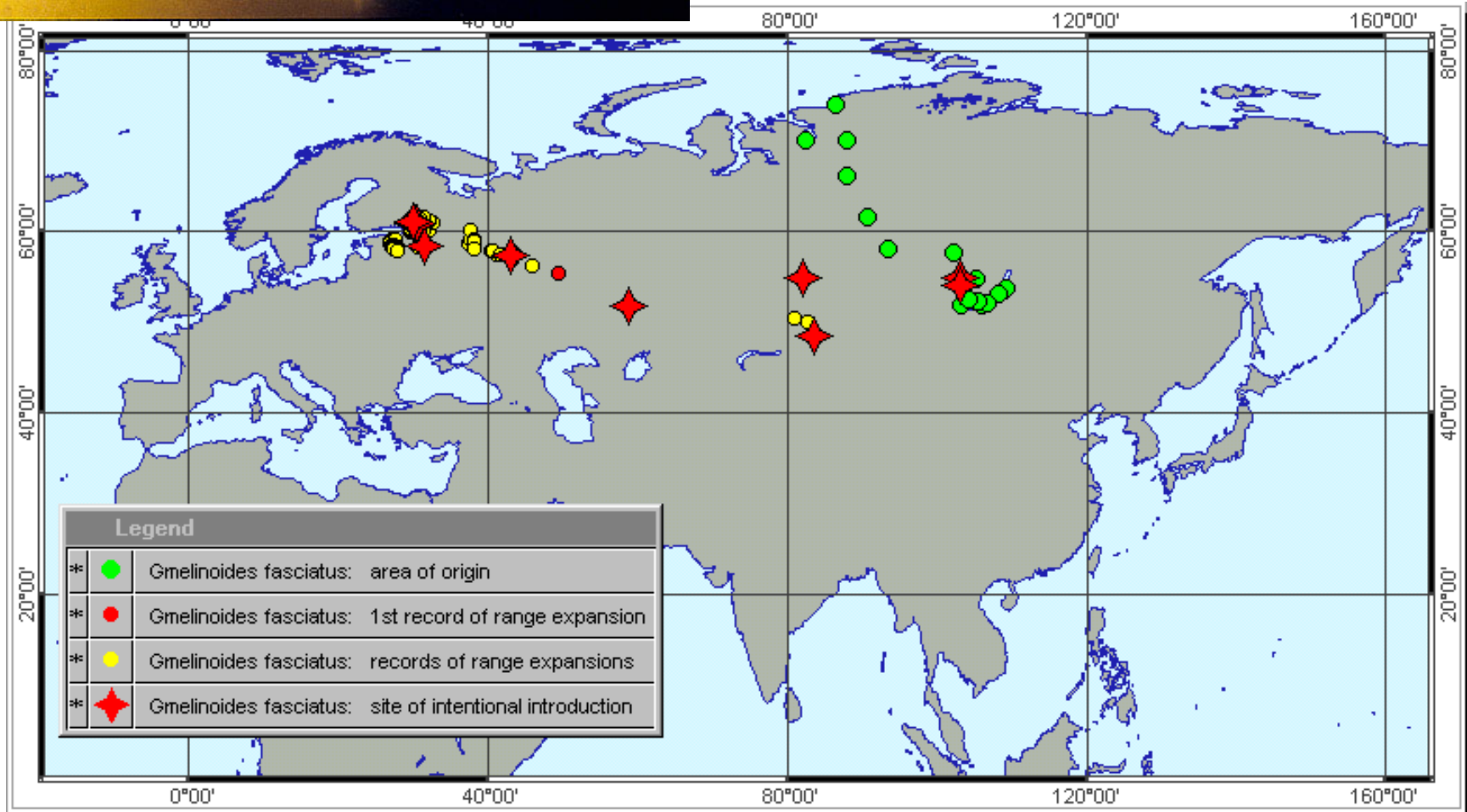
In Lake Baikal there are no strict specialists, at least close to surface, where impact of environmental changes is more dramatic.

Are there specialists in the abyssal zone? It is not yet known, but this zone is relatively young.

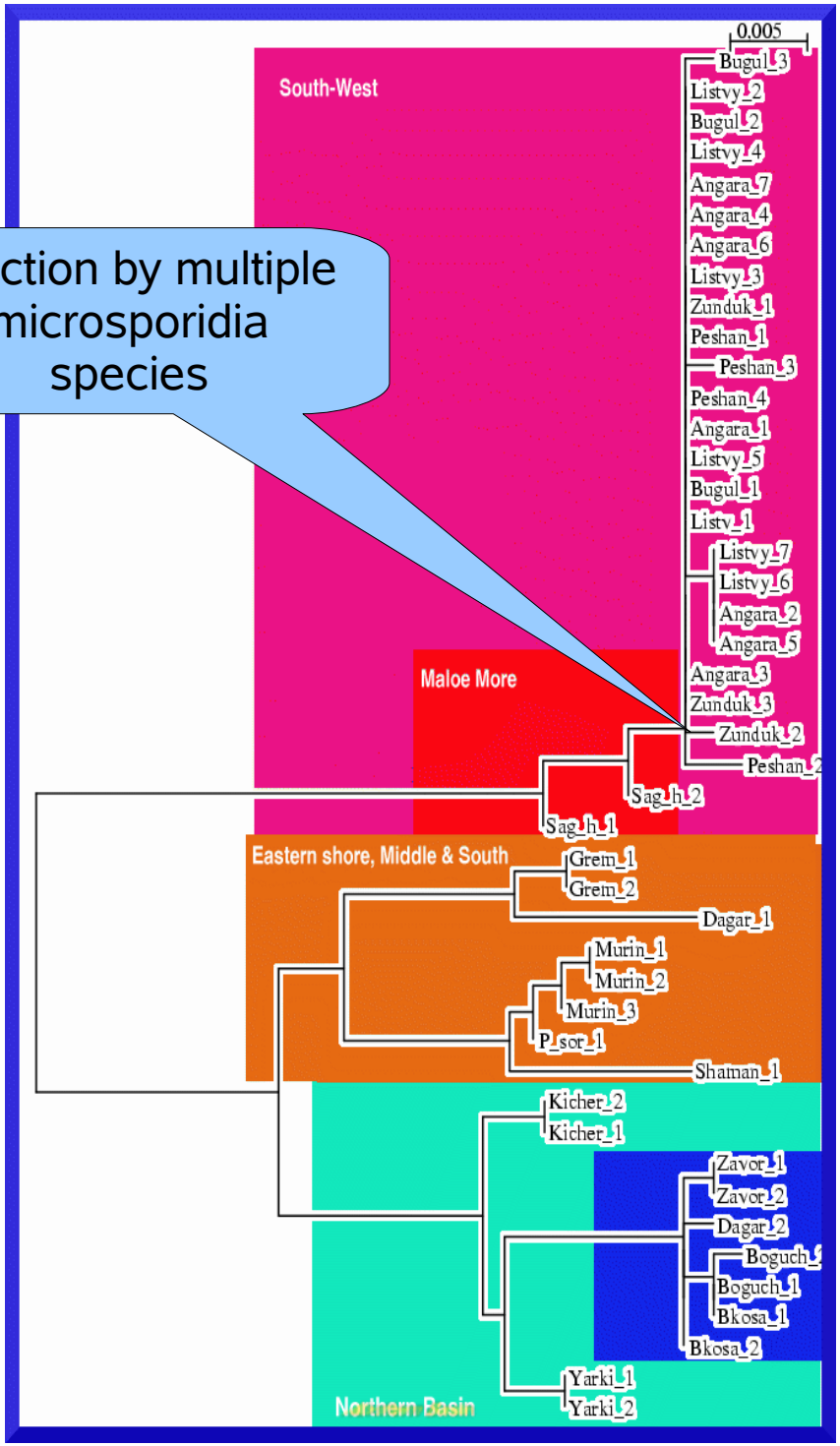
Shackleton cycles: evolution in changing environment



Subdivision in *Gmelinoides fasciatus*
(Environmental changes are not the only cause of species subdivision)



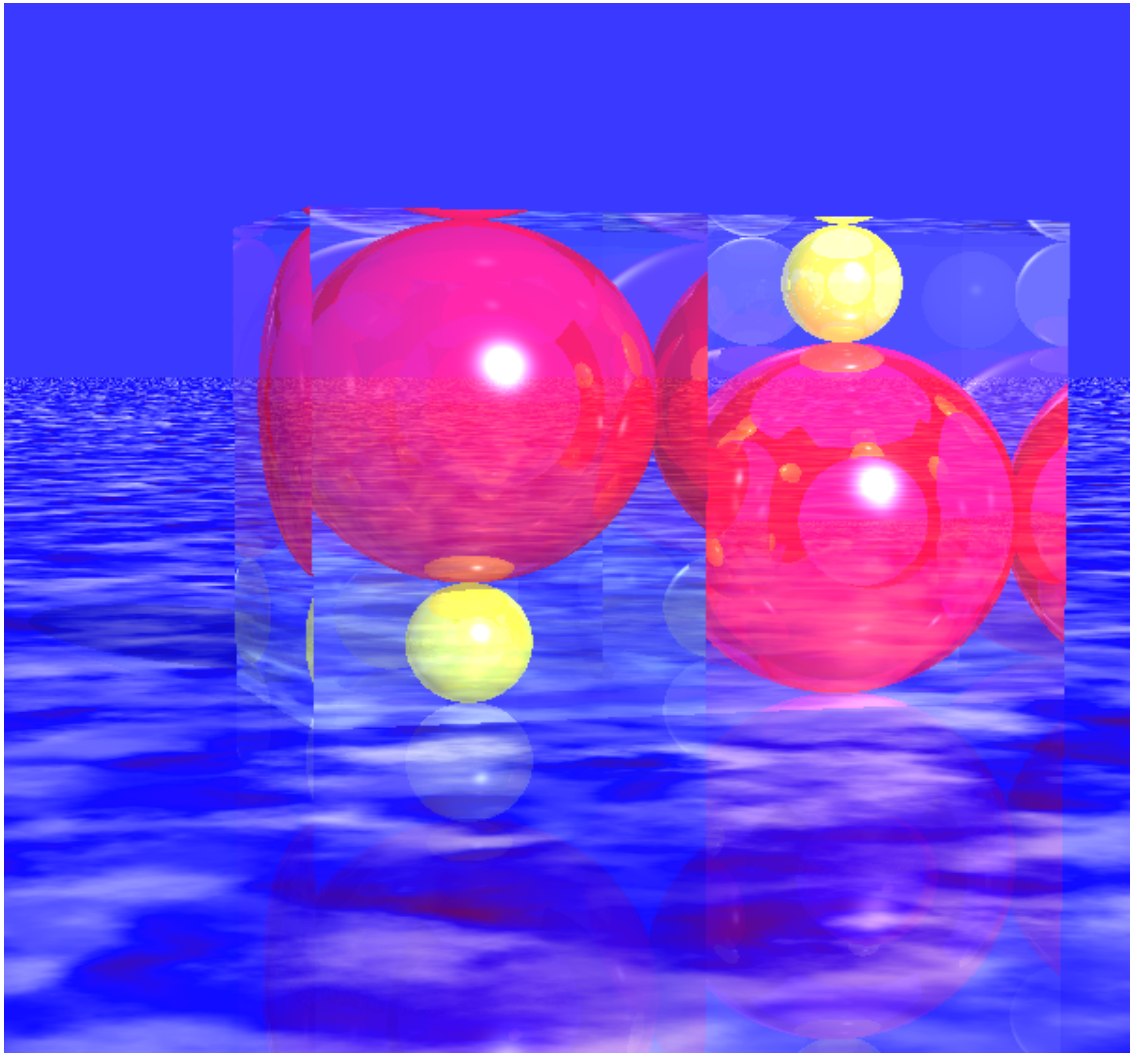
Are different populations separate species?
How could this pattern occur?



Coordinated evolution of amino acid sequences

Some features of proteins preserved in evolution involve more then single amino acid residue

- There is no obvious transition from one state to another: intermediate state is deleterious
- Numerous physical or/and chemical properties of amino acid residues may be conserved,as the consequences the values of these properties appear to be highly correlated in evolution
- More then two residues may take part in a group
- Correlated groups are quite common in proteins



Objectives:

- To elucidate the population mechanism allowing coordinated evolution of amino acid residues;
- Using computer simulation of microevolutionary events, to find the conditions favouring coordinated evolution
- To design statistical tests allowing one to study coordinated evolution or/and take it into account when necessary

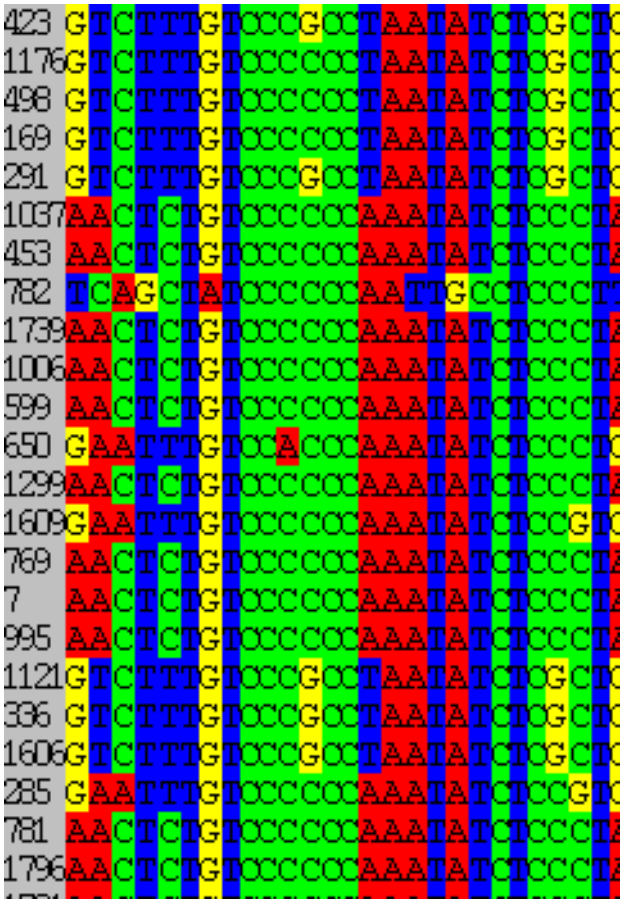
Model

Organism

- Hermaphroditic, but during the same reproduction cycle may have only one gender
- Diplod and has maternally transferred («mitochondrial») DNA
- Has age limit measured in reproductive cycles
- Fitness depends on one protein coding gene and population density limited resource)
- Number of progeny is Poisson distributed

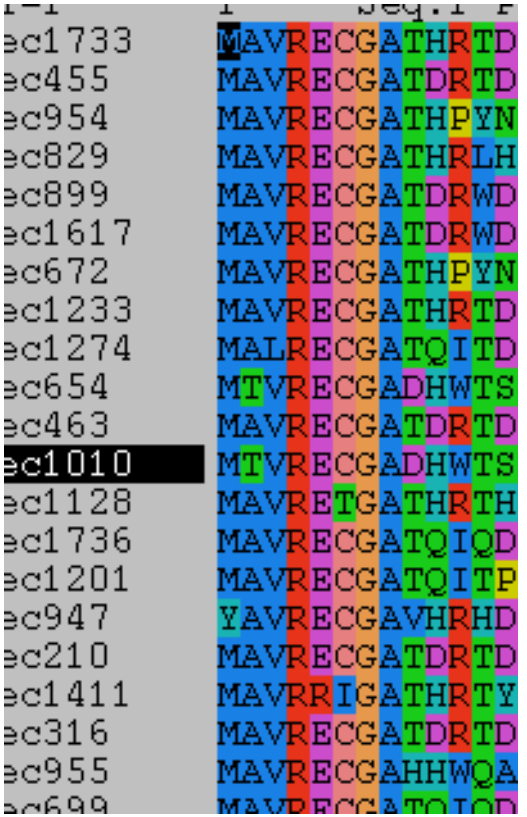
Mitochondrial marker

- Single vector $x_i \in A, C, G, T$
- No recombination
- Transfered from mother to all her progeny
- Does not affect fitness
- All substitutions (mutations) are equiprobable



Model

Nuclear gene



- Sequence consists of 20 «amino acids»
- Each substitution is equiprobable;
- Each residue has property, which changes from 0 to 19
- Each sequence consists of 2 parts: «the neutral one, where sequences does not affect fitness of the organism, and **non-neutral one,**where fitness is function of the sum of properties:

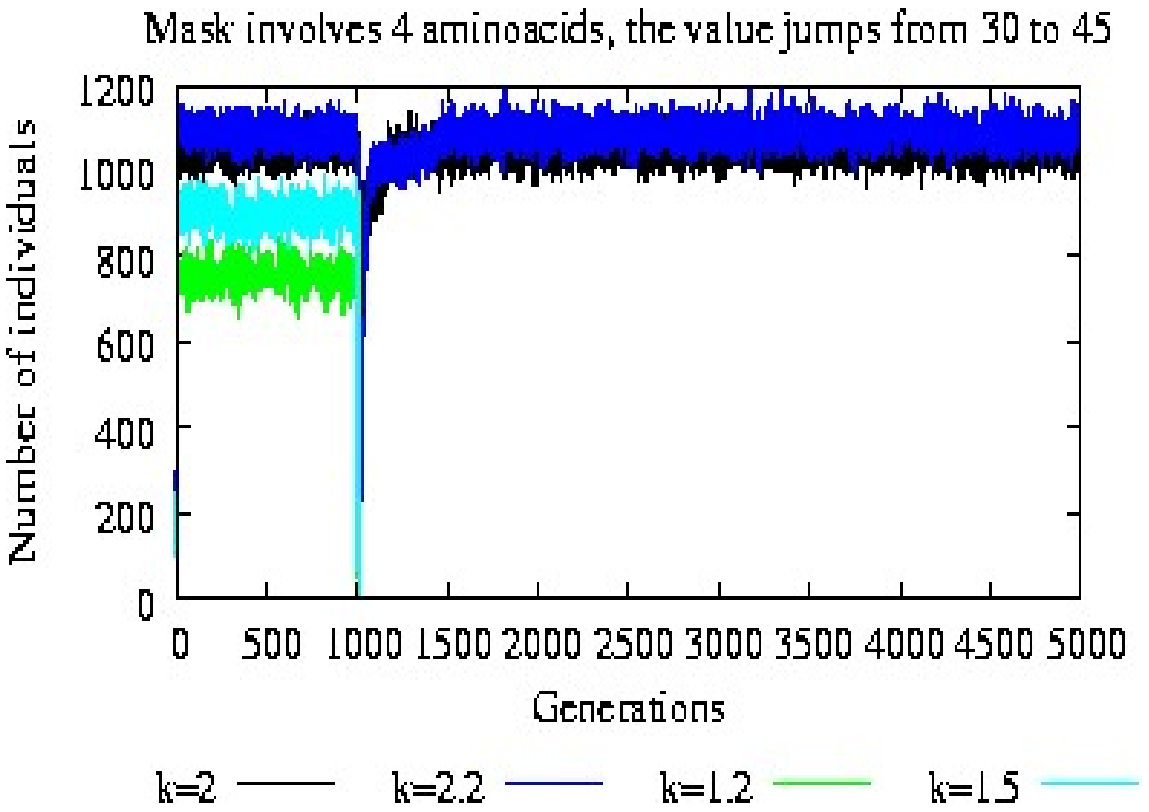
$$f = \sum \left(x_i - s_i \right)$$

Interactions between organisms

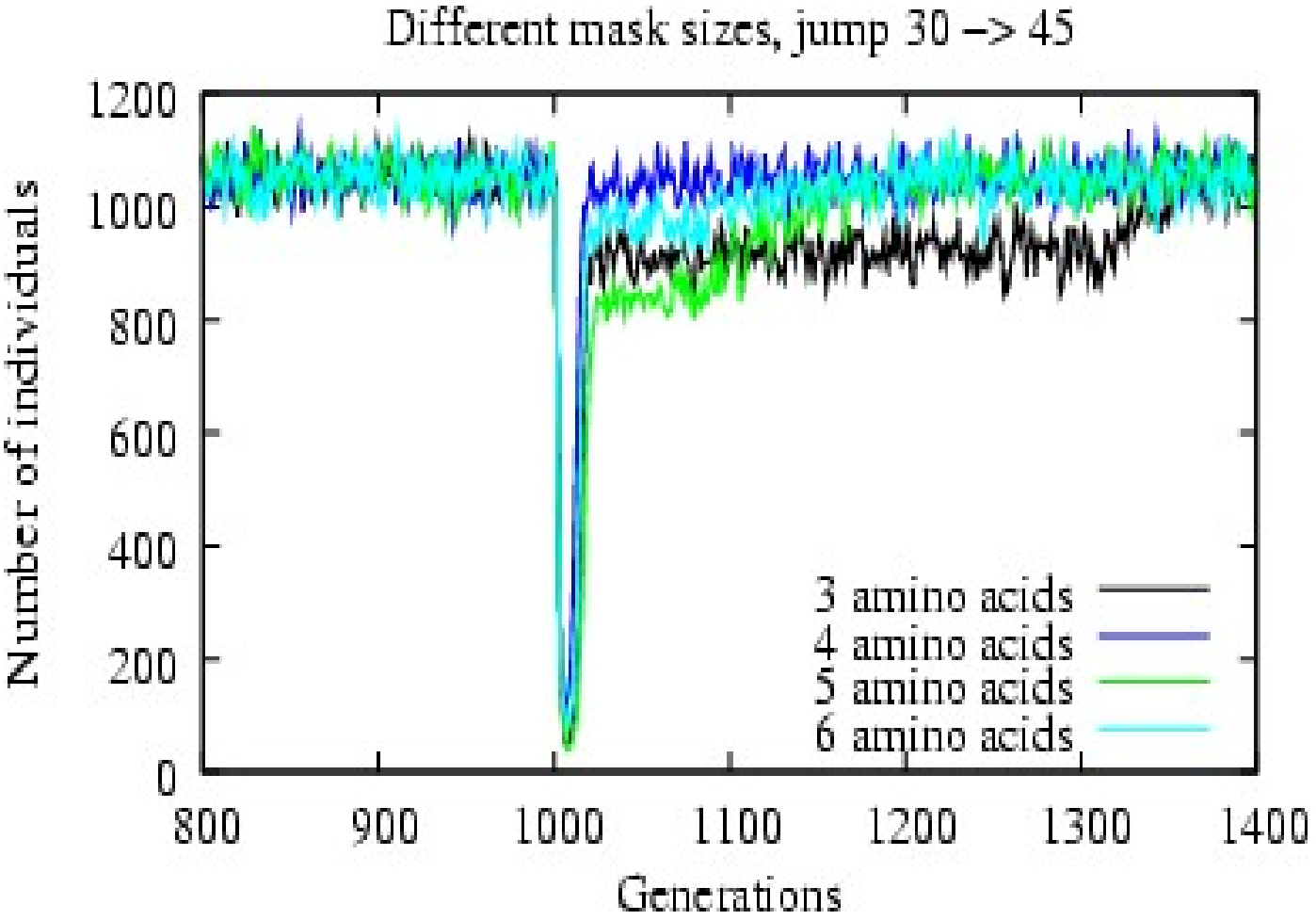
$$f = f\left(1 - \frac{n}{N}\right)$$

1) The organisms who reached maximal age allowed die;
2)Each of the survivors determine it's gender for this round;
3)Density-dependent decrease of survival rate is introduced;
4)Pairs («families» are formed according to the random gender-choice made at stage (2);
5)Each pair «decides» how many children will they have. The number of children is Poisson-distributed;
6) Children are produced (if their number exceed the max. Number, their number is reduced proportionally), They inherit mother's «mitochondrial» marker and one «nuclear» allel from each parent;
7)Progeny fitness according to the group rule is calculated (Full dominance in this study)
8)New density dependent viability is calculated and the unlucky «die», the rest increase their age;
9)Stage (1) occurs. Life goes on.

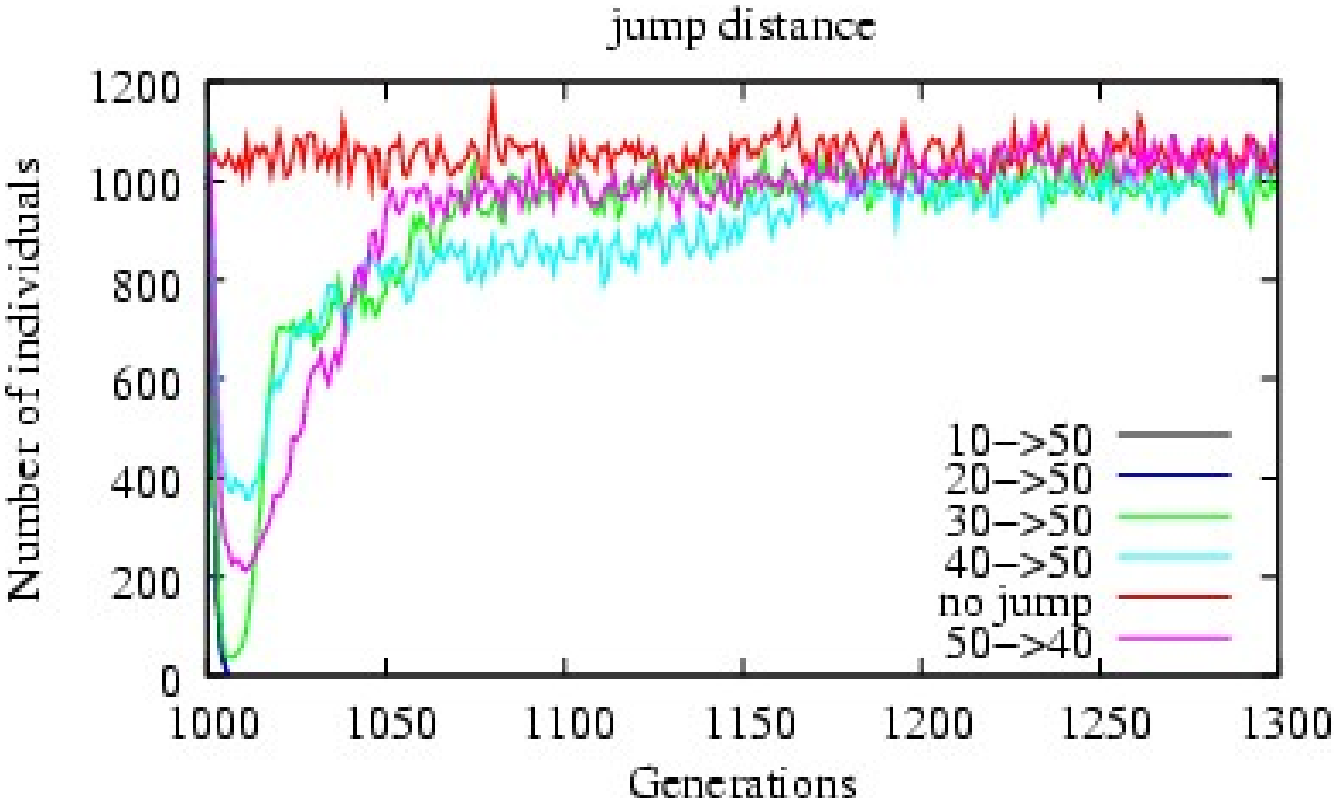
Mask size, number of kids etc.

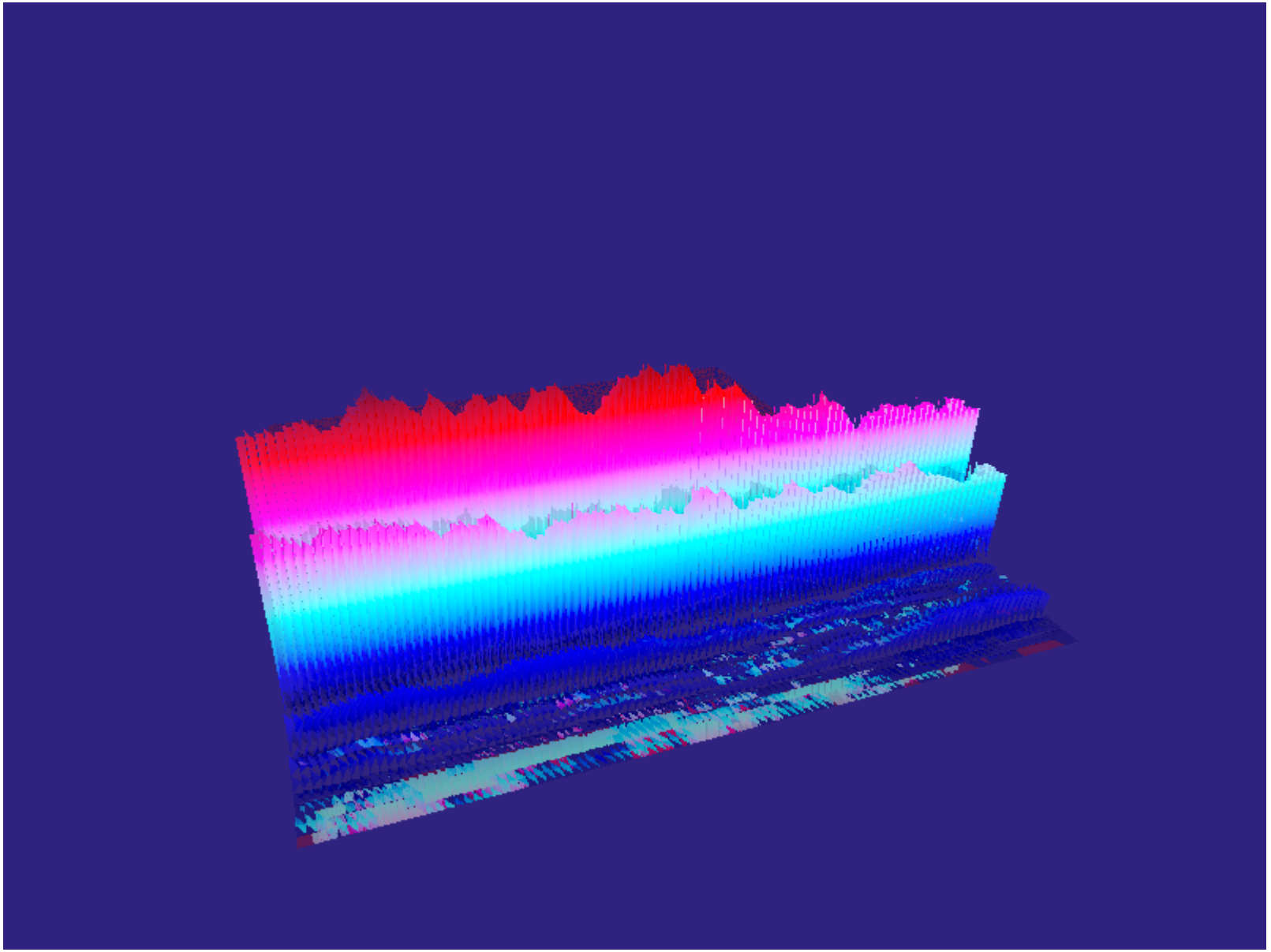


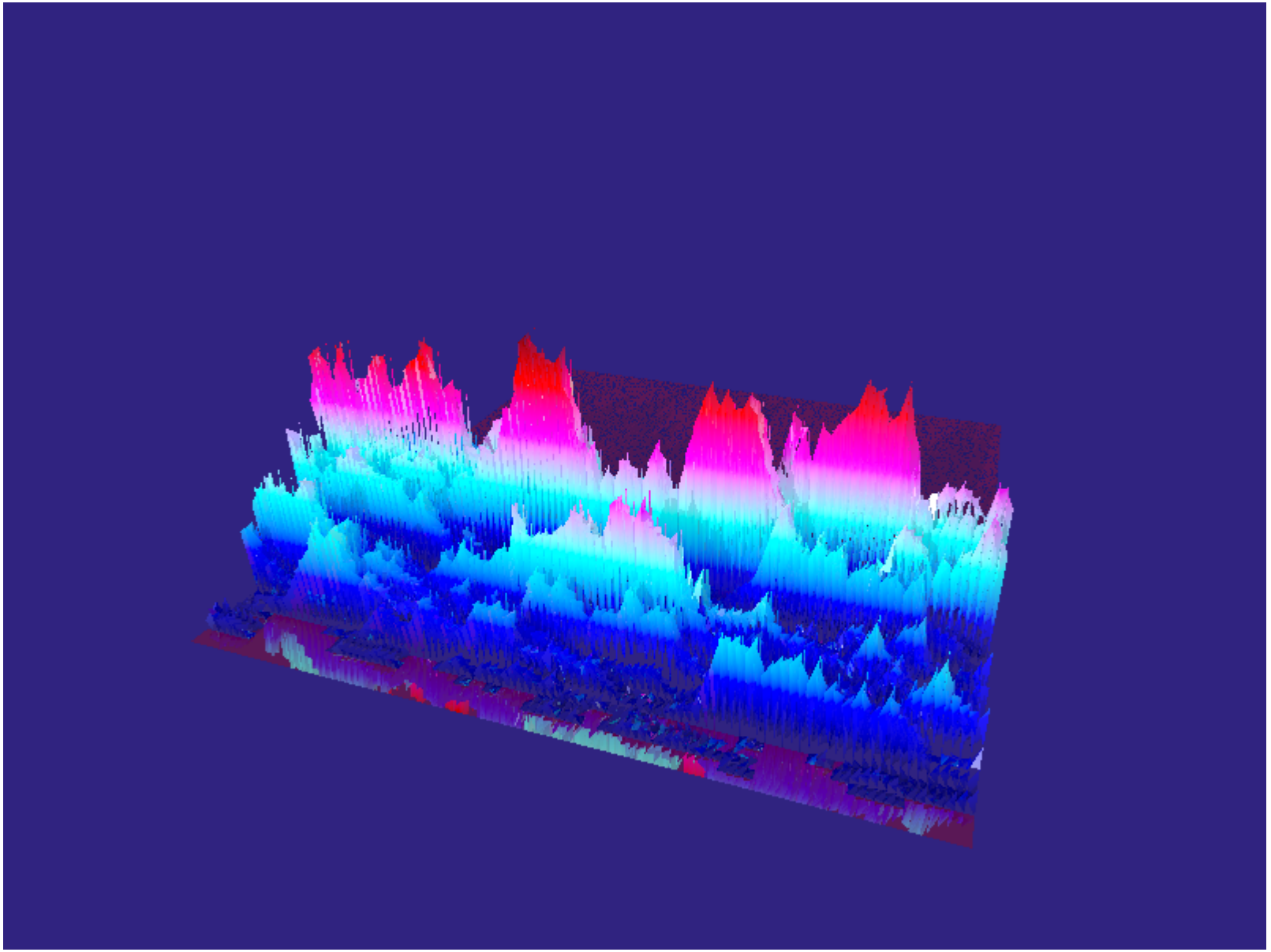
Group size influences relaxation curve after a jump



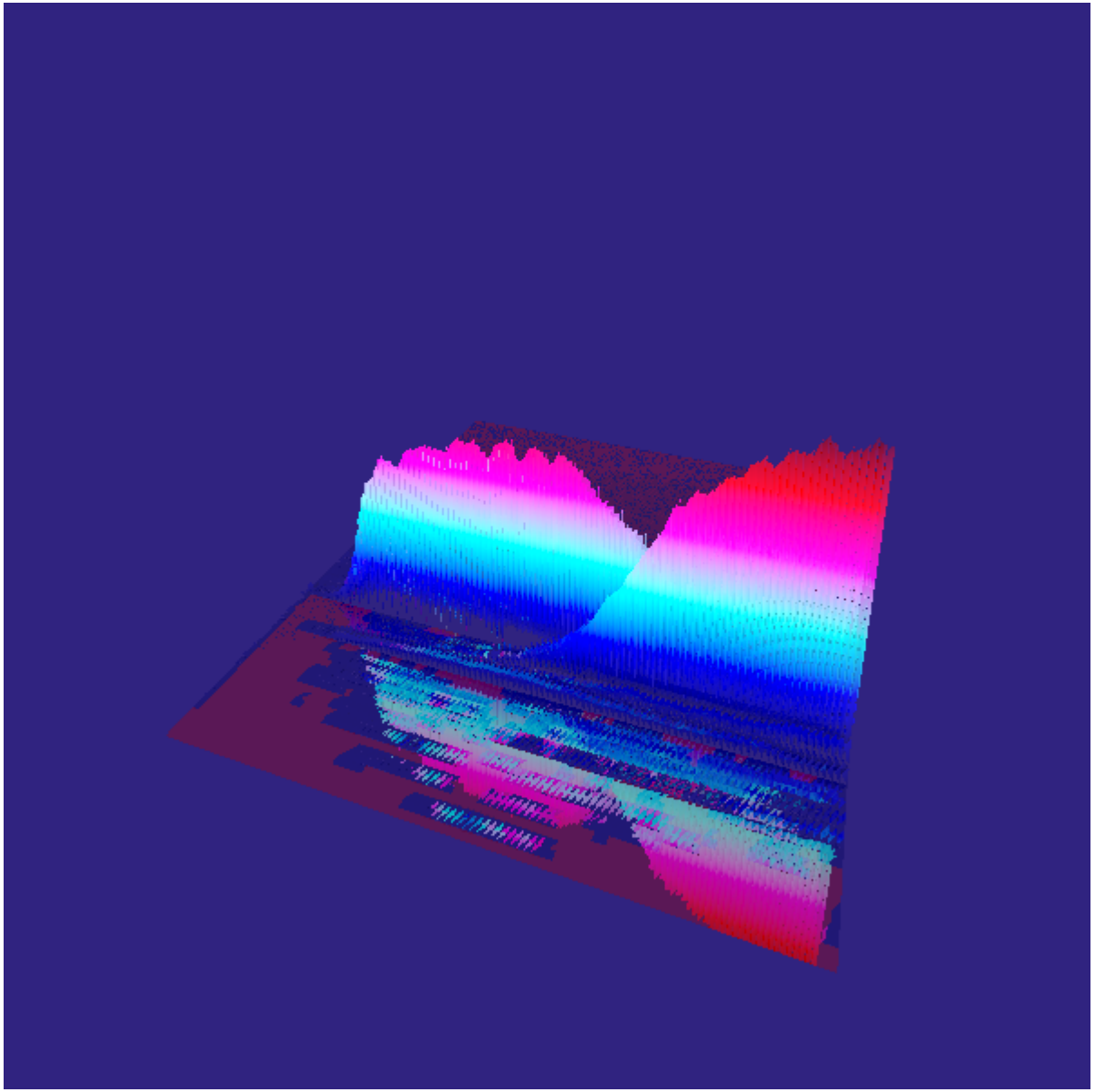
Relaxation curves depend on exact start and target values



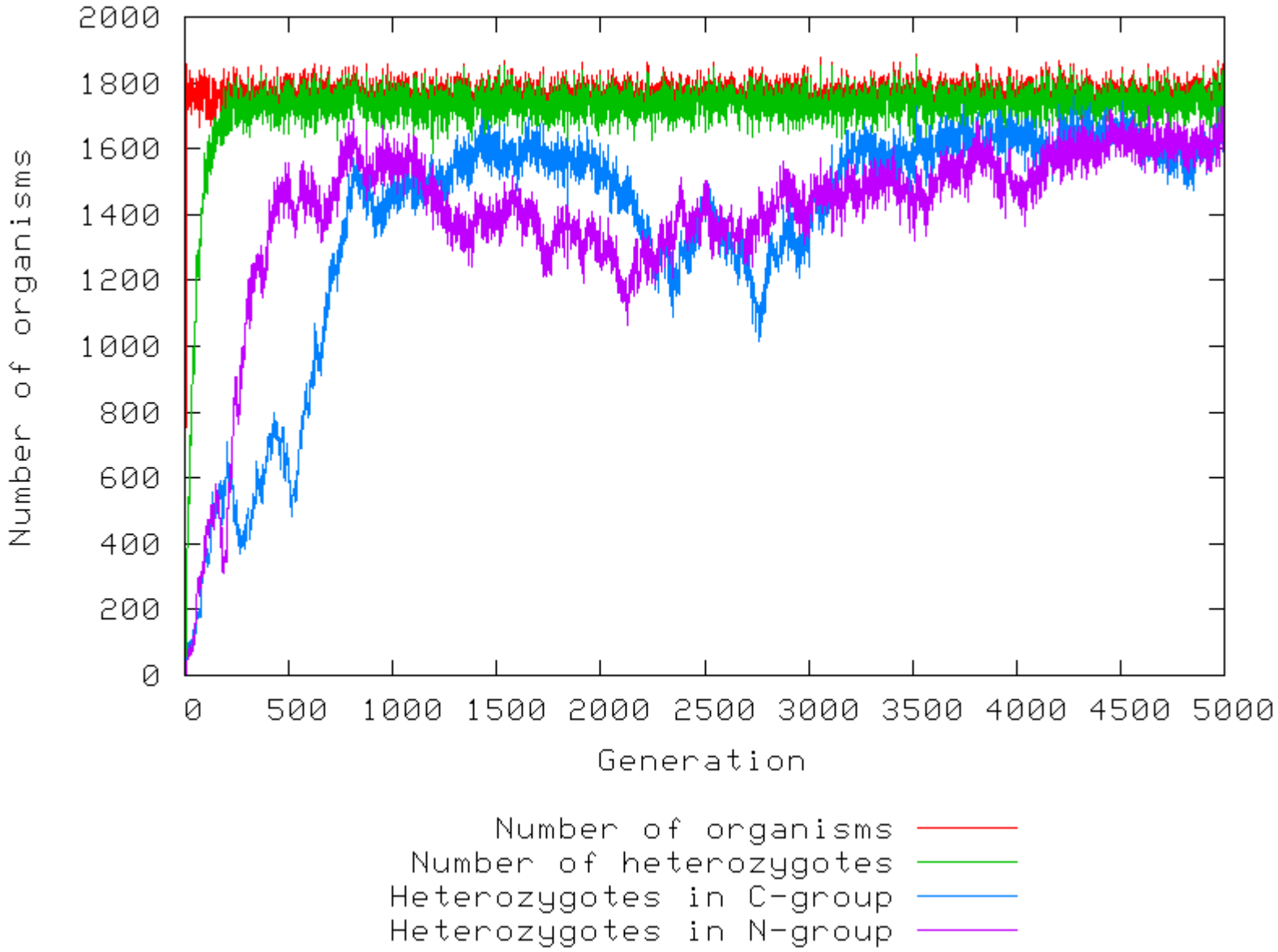




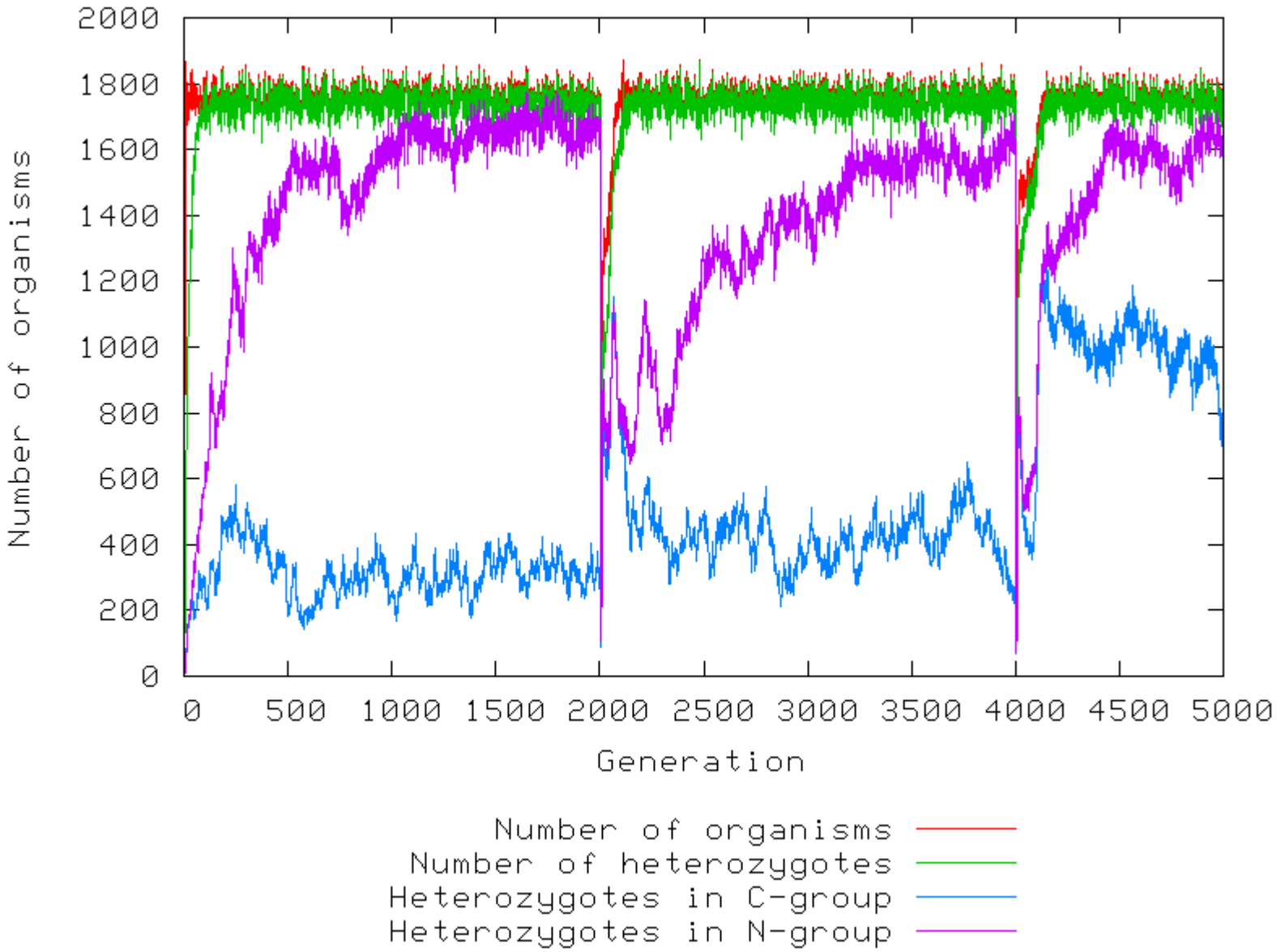
Optimum shift without coordinated evolution

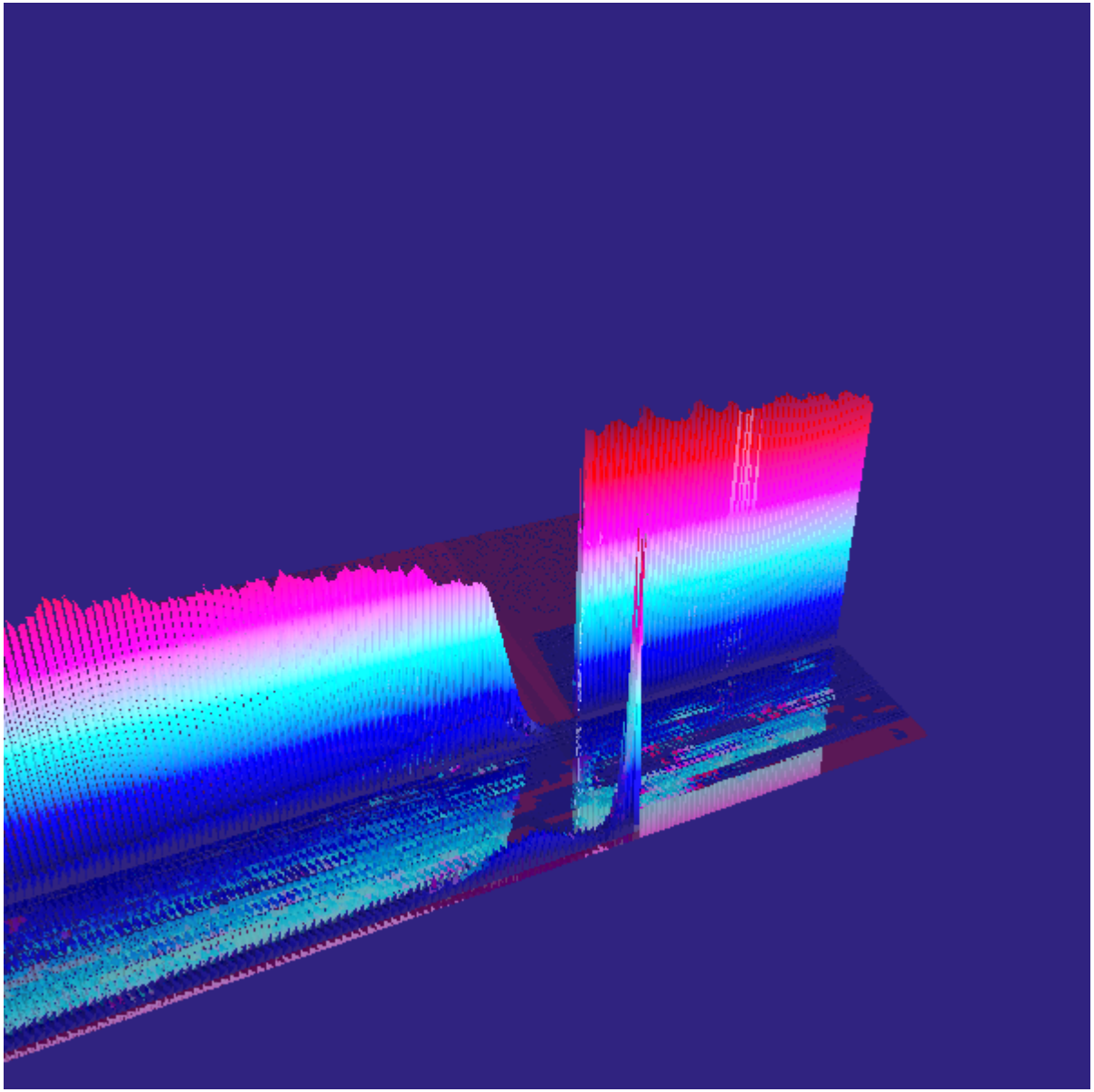


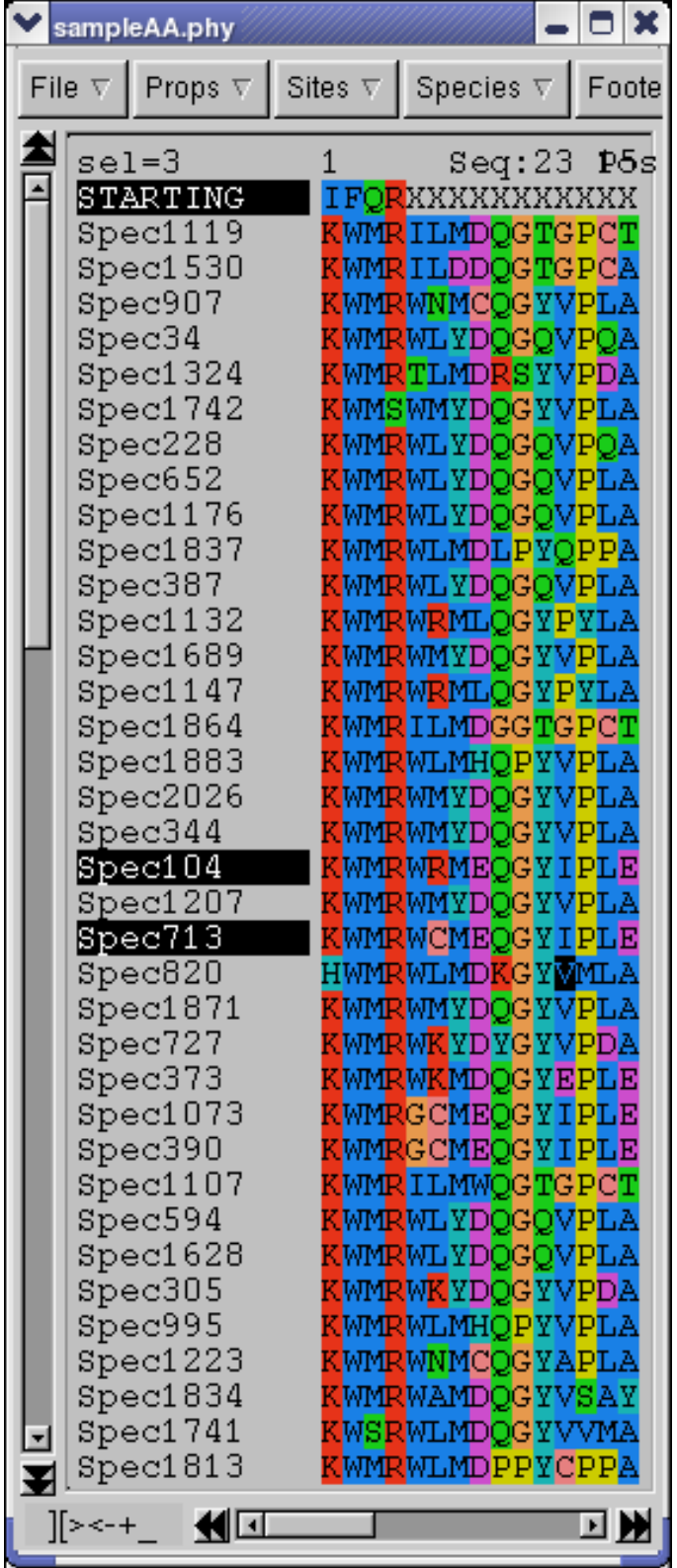
Two optinmal values co-existing do not cause co-ordinated substitutions



Double jump

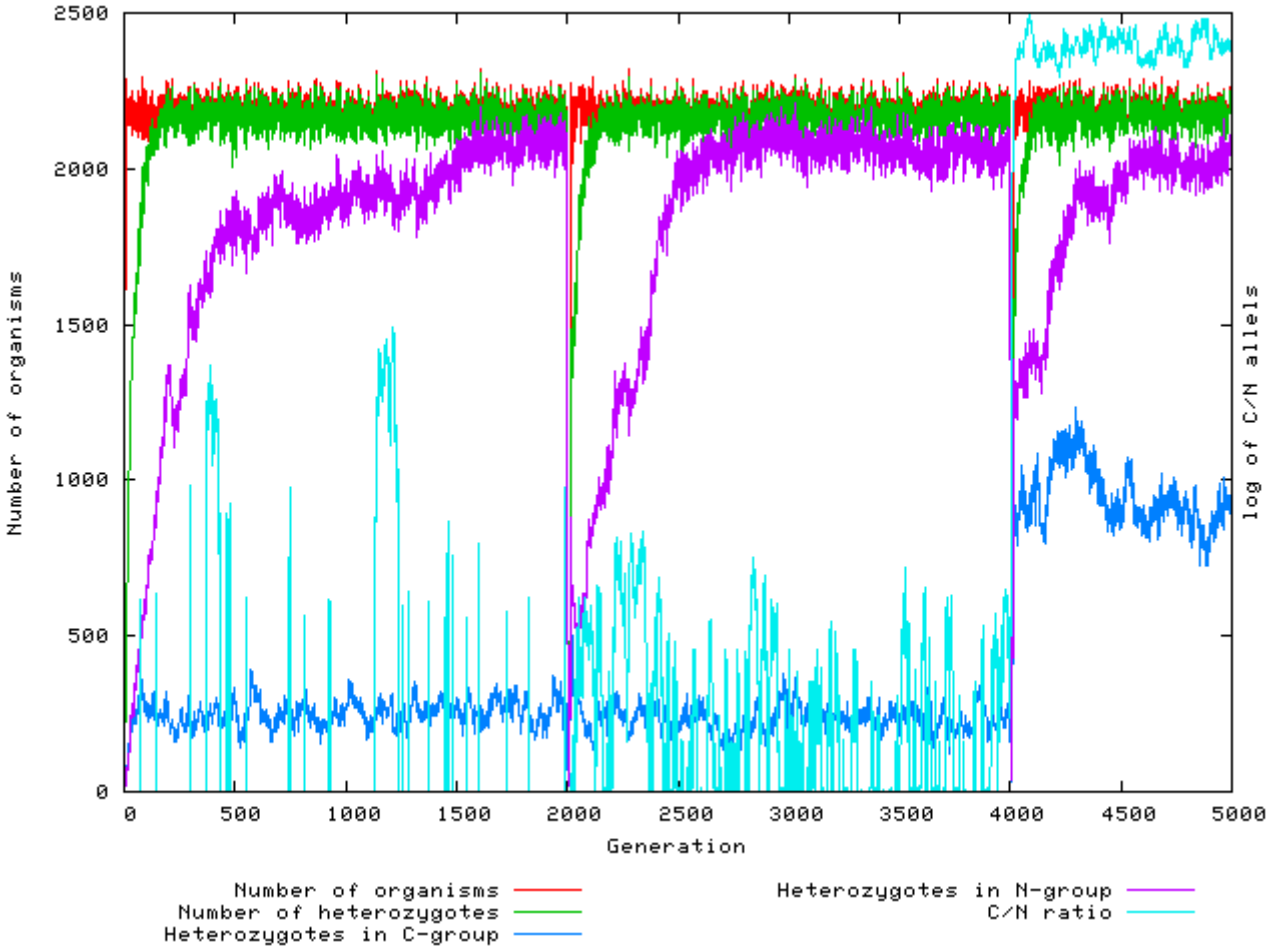

Number of organisms
2000
1800
1600
1400
1200
1000
800
600
400
200
0
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
Generation
Number of organisms
Number of heterozygotes
Heterozygotes in C-group
Heterozygotes in N-group





Double shift of optimal value results in coordinated sunstitutions!

Repeated change of environment promotes coordinated substitutions



Very preliminary conclusions:

- *Number of group members must be more then 2. Coordinated substitutions become more frequent with the increase of number of group members.*
- *Periodic shift of optimim promotes coordinated substitutions*
- *New optimal value of a property must be reached at a single mutation*