Supplementary Information for

Mito-nuclear selection induces a trade-off between species ecological dominance and evolutionary lifespan

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Contents

S1 Diversification rates

In this section we show how the diversification rates – speciation, hybridization and extinction – depend on the selection strength at equilibrium and how they behave along the evolutionary process (radiation and equilibrium).

Figure S1 shows the diversification rates per species in the equilibrium regime for different selection strengths σ_w and in the absence of selection (non-interacting case, NI) (analogous to the rate of speciation per lineage, as usually shown for comparison of latitudinal gradients [1]). We note that the number of species in equilibrium varies considerably with σ_w (Fig. 2b of the main text). Figure S2 show the diversification rates along the evolutionary time (instantaneous rates evaluated for time bins $\Delta t = 10$ generations), displaying peaks during the radiation and reaching a steady state afterwards. The net diversification rate, result from speciation minus extinction and hybridization, peaks at the radiation and it is null in the equilibrium, when species richness reaches a plateau.

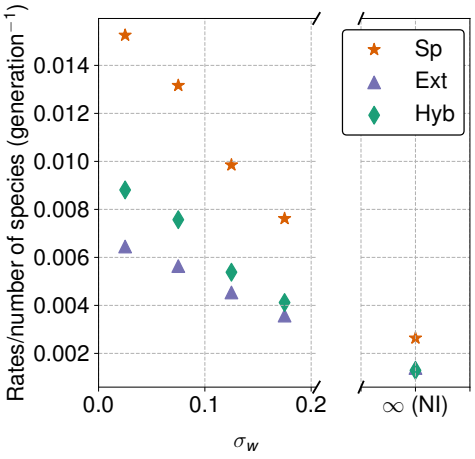

Figure S1: Diversification rates per species in the equilibrium: speciation (Sp), extinction (Ext) and hybridization (Hyb).

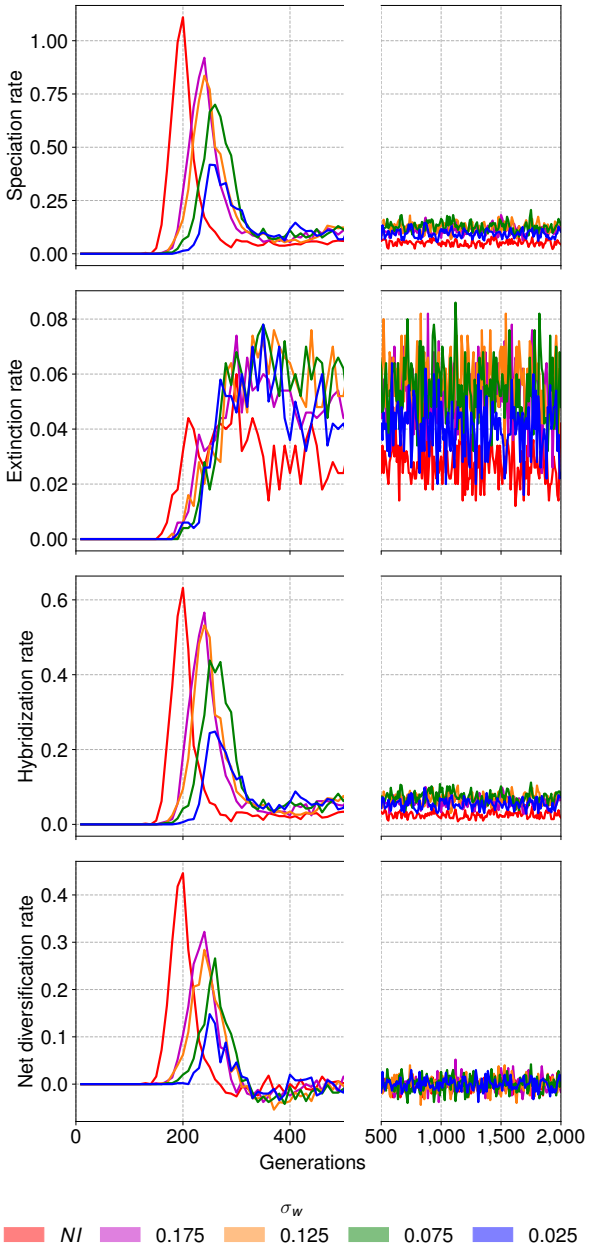

Figure S2: Diversification rates over time. Events were accumulated over time intervals $\Delta t = 10$ and the results divided by Δt.

S2 Scalability of the community size

Our simulations resulted in a small number of species in equilibrium. In order to obtain good statistics for the species abundances distributions (SAD), we have accumulated the results of several independent simulations. To validate this methodology, we compared the resulting distributions for each value of σ_w with a single simulation of a large population of $M = 20,800$ individuals keeping the demographic density constant, i.e., expanding the area to a 400×400 lattice. Figure S3 shows the accumulated result over 50 simulations, comprising $\sim 65,000$ individuals (Fig. S3a), accumulated results over 16 simulations with a total of $\sim 20,800$ individuals (Fig. S3b) and single simulation with 20,800 individuals (Fig. S3c). Variation of the number of individuals are due to stochastic fluctuations in mating choice during the simulations. We observed that the SADs were equivalent regarding the number of species sampled and the average species abundance.

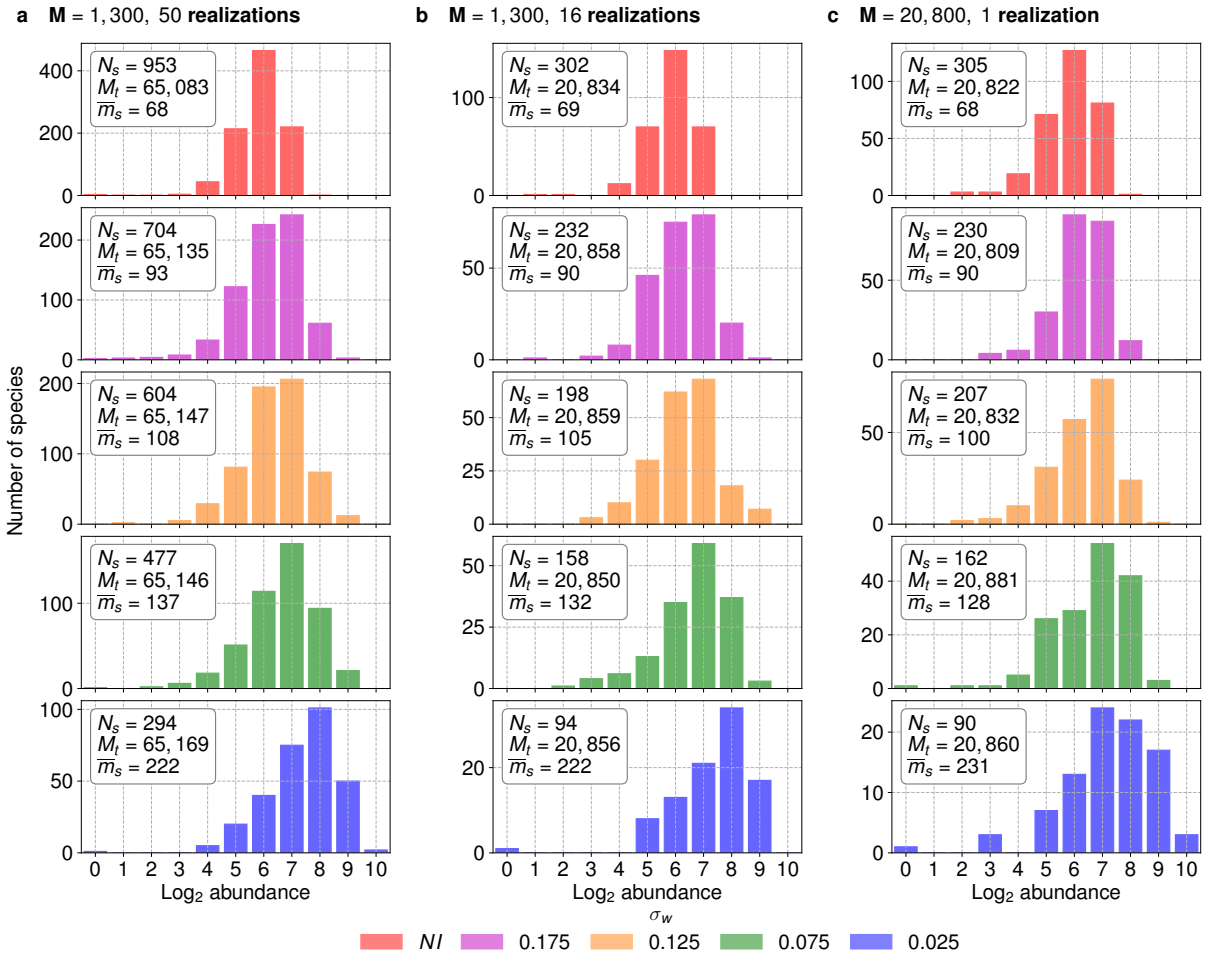

Figure S3: Species abundances distributions accumulated over 50 simulations with 1,300 individuals (a); over 16 simulations with 1,300 individuals (b); and single simulation with 20,800 individuals (c).

S3 SADs at intermediary times

Here we show that, after equilibration at $T \approx 500$ generations, the abundances distributions do not change significantly, reaching a steady configuration. Figure S4 shows that, despite small fluctuations due to the stochastic nature of the model, the overall shape of the distributions do not change.

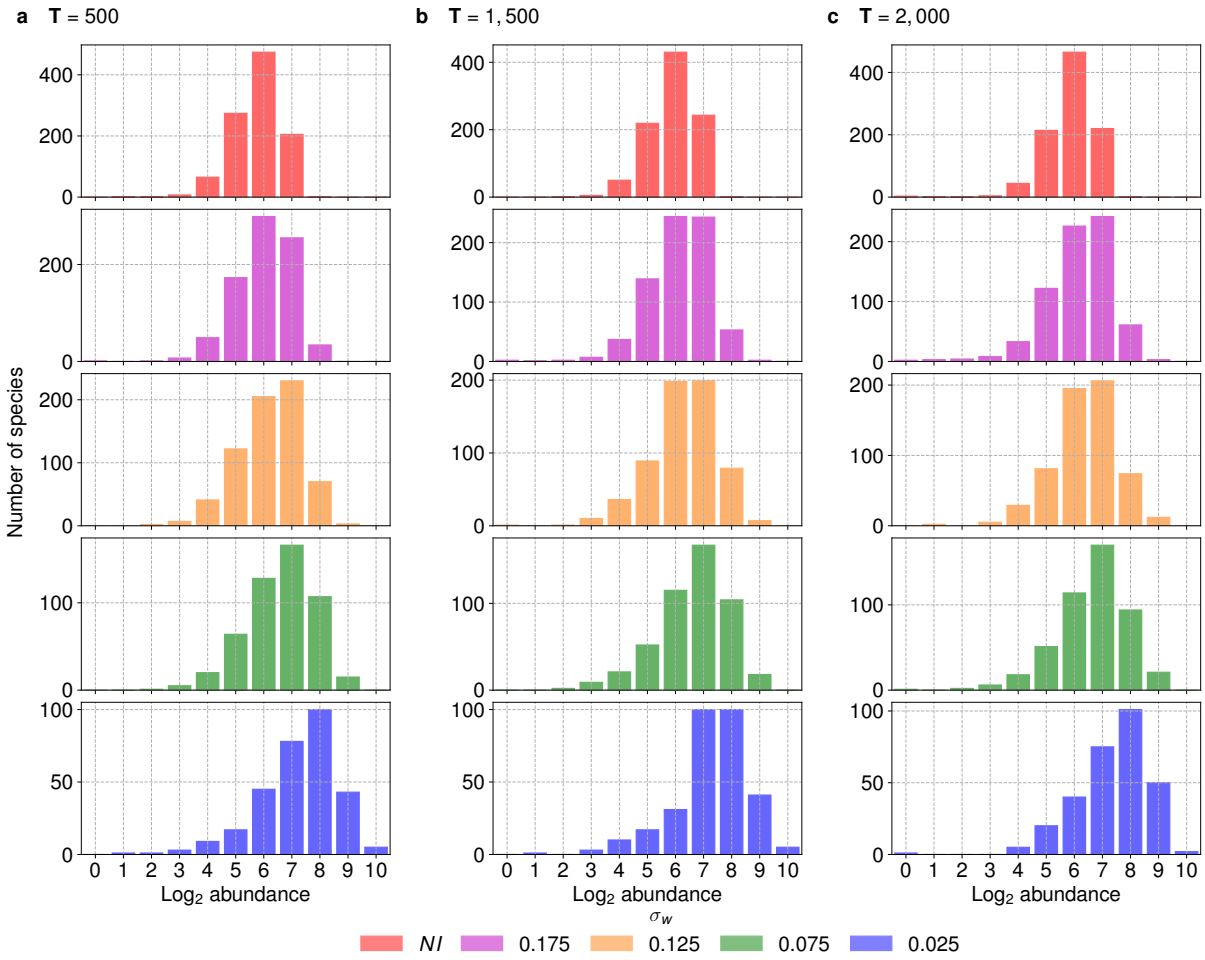

Figure S4: Abundance distributions computed at three different times after the radiation period. Although small fluctuations are observed, the overall shape does not change significantly over time.

S4 Species' ages and time for death

Here we investigate how species abundances correlate with age at the time of sampling and remaining lifetime. Species were detected at $T = 1,000$ and their abundances and ages computed. Figure S5 shows that species of intermediate sizes are older (Fig. S5a) and live longer (Fig. S5b) when selection over the mito-nuclear interaction is considered. The non-interacting case shows no significant correlation between lifespans and abundances, except for small species, that tend to go extinct faster.

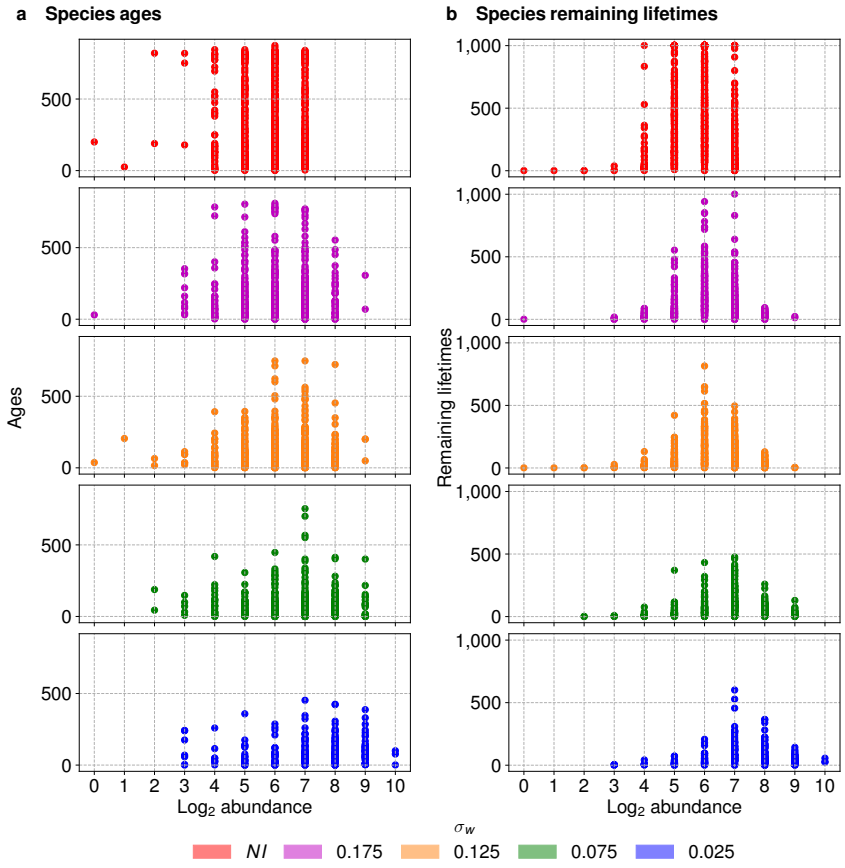

Figure S5: Relation between species abundances and their (a) ages and (b) and remaining lifetimes for species extant at $T = 1,000$.

S5 Mitochondrial distances

Figure S6 shows the distribution of mitochondrial distances between (Fig. S6a) and within (Fig. S6b) species. Selection over mito-nuclear interaction drastically reduces the interspecies distances, implying in more genetically similar species. Intraspecies distances, on the other hand, change from an exponential distribution with large average distance (non-interacting case) to a unimodal distribution with much smaller average distance. Species, therefore, become more uniform in terms of their mitochondria as selection strength increases. For the mitochondrial DNA, which does not recombine and is not under mating restriction, selection utterly increased similarity within species, spontaneously forming clusters of mitochondria (Fig. S6b).

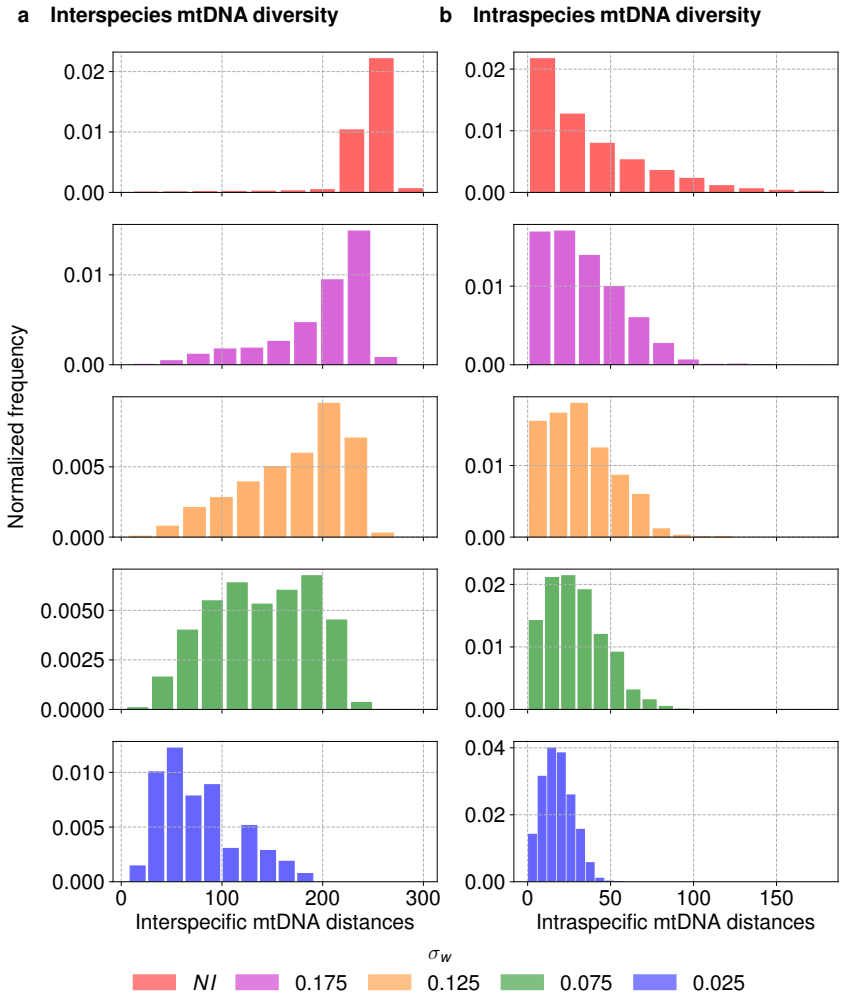

Figure S6: Mitochondrial distances between pair of individuals belonging to different species (a) and from the same species (b). Similarly to the nDNA, mito-nuclear selection reduced the mitochondrial distances between individuals of different species. For individuals of the same species, the mtDNA distances also reduced with selection, in opposite trend to the nDNA.

S6 Substitutions rates

In our simulations the mutation probabilities per locus were fixed at $\mu = 0.00025$ for the nDNA and $\mu_M = 0.00075$ for the mtDNA. Mutation reversals, however, decrease the effective number of mutations and selection filters out 'deleterious' mutations that decrease fitness, also decreasing the net rate of substitutions.

The number of substitutions is computed as the number of loci that changed from the initial state 0 to state 1 at $T = 2,000$. For the non-interacting case, the probability that a single mutation occurs and is not reversed after T generations is $\binom{T}{1}\mu(1-\mu)^{T-1}$. The probability that a mutation occurs and is reversed twice is $\binom{T}{3}\mu^3(1-\mu)^{T-3}$. Thus, $\mu[(1-\mu)^{T-1} + \frac{(T-2)(T-1)}{6}\mu^2(1-\mu)^{T-3}]$ is an estimate for the average number of substitutions per generation. The expected substitution rates of the nuclear and mitochondrial genomes in the non-interacting case are then 1.5×10^{-4} and 2.3×10^{-4} per generation, respectively [2].

Figure S7a shows the substitution rate per locus in the mtDNA in the non-interacting case (red) and the strongly interacting case (blue). Figure S7b shows similar information for the nDNA, separated into coupled sites (first 500 loci) and uncoupled sites (remaining 1,000 loci).

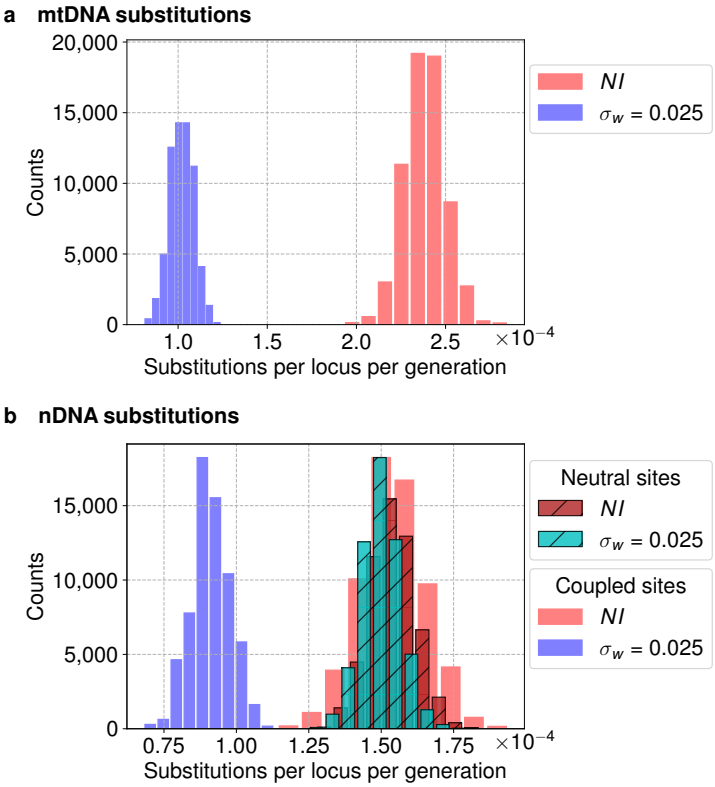

Figure S7: Substitution rates per locus per generation for the mtDNA (a) and for the nDNA (b).

References

1. Schluter, D. & Pennell, M. W. Speciation gradients and the distribution of biodiversity. *Nature* **546**, 48–55 (2017).

2. Princepe, D. & De Aguiar, M. A. M. Modeling Mito-nuclear Compatibility and Its Role in Species Identification. *Systematic Biology* **70**, 133–144 (2021).