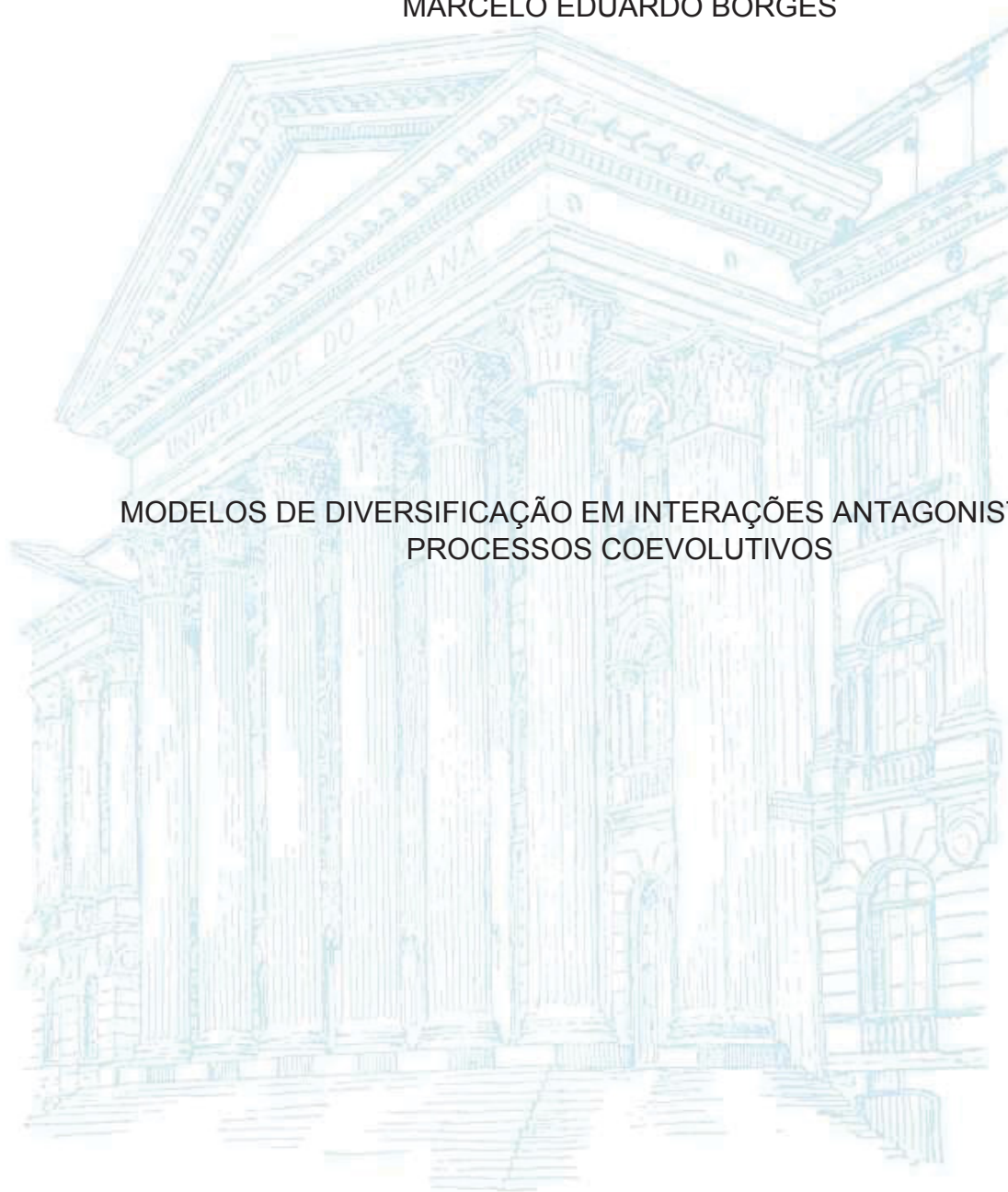


UNIVERSIDADE FEDERAL DO PARANÁ

MARCELO EDUARDO BORGES

MODELOS DE DIVERSIFICAÇÃO EM INTERAÇÕES ANTAGONISTAS VIA
PROCESSOS COEVOLUTIVOS



CURITIBA

2020

MARCELO EDUARDO BORGES

MODELOS DE DIVERSIFICAÇÃO EM INTERAÇÕES ANTAGONISTAS VIA
PROCESSOS COEVOLUTIVOS

Tese apresentada ao curso de Pós-Graduação em Ecologia e Conservação, Setor de Ciências Biológicas, Universidade Federal do Paraná, como requisito parcial à obtenção do título de Doutor em Ecologia e Conservação.

Orientadora: Profa. Dra. Sabrina Borges Lino Araújo

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À minha família,
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“Science is what we understand well enough to explain to a computer.

Art is everything else we do.”

Donald E. Knuth

RESUMO

Esta tese estuda o papel de processos coevolutivos em interações antagonistas na diversificação das espécies. Interações antagonistas se referem a qualquer interação entre espécies no qual uma espécie é beneficiada em detrimento da outra, podendo se referir a interações parasito-hospedeiro, parasitóide-hospedeiro e herbívoros-planta. É utilizada uma abordagem de simulações computacionais e modelos baseados em indivíduos de modo a servir como “prova de conceito” de hipóteses teóricas a respeito de processos coevolutivos. No capítulo 1, eu faço uma breve introdução a respeito de coevolução, interações antagonistas e o Paradigma de Estocolmo, que serve como referencial teórico para os modelos desenvolvidos nos próximos capítulos. No capítulo 2, eu avalio como interações antagonistas em um par de espécies são influenciados por estratégias de reprodução sexuada e asexuada. Os resultados deste trabalho demonstram que para modelos de fenótipos quantitativos que consideram genomas com múltiplos loci de forma explícita, a estratégia reprodutiva resulta em dinâmicas coevolutivas distintas. Enquanto modelos com reprodução asexuada podem resultar em bifurcações evolutivas ou extinção do consumidor, modelos de reprodução sexuada resultam em oscilações e interações persistentes. No capítulo 3, eu estudo como a interação com diferentes recursos afetam a evolução do tamanho do repertório de hospedeiro e a riqueza de espécies em um modelo espacialmente explícito. É demonstrado que ao se considerar aspectos geográficos e a seleção devido ao uso de recursos simultaneamente, as linhagens oscilam o seu grau de especialização ao longo de múltiplos eventos de especiação, conforme previsto pela Hipótese da Oscilação. Ao mesmo tempo, pressões seletivas mais intensas e menor capacidade de dispersão atuam conjuntamente para produzir maior riqueza de espécies. Estes trabalhos ilustram através de diferentes maneiras em como o estudo de processos coevolutivos pode nos ajudar entender melhor dinâmicas de coexistência das espécies à geração da biodiversidade.

Palavras-chave: Parasito-hospedeiro. Interações ecológicas. Coevolução. Especiação. Diversificação.

ABSTRACT

This thesis investigates the role of coevolutionary processes in antagonistic interactions in the diversification of species. Antagonistic interactions refer to any interaction between species in which one species benefits at the expense of another and can refer to either parasite-host, parasitoid-host and herbivore-plant interactions. I use an approach of computational simulations and individual-based models to apply a “proof of concept” on theoretical hypotheses regarding coevolutionary processes. In chapter 1, I present a short introduction about coevolution, antagonistic interactions and the Stockholm Paradigm, which is the underlying theoretical framework for the models developed in the following chapters. In chapter 2, I assess how antagonistic interactions in a pair of species are influenced by sexual and asexual reproductive strategies. This paper demonstrates that for models of quantitative traits that consider genomes with multiple loci explicitly, the reproductive strategy results in distinct coevolutionary dynamics. While models with asexual reproduction may result in evolutionary branching or consumer extinction, models of sexual reproduction result in oscillations and persistent interactions. In chapter 3, I study how the interaction with different resources affects the evolution of host range and species richness in a spatially explicit model. I demonstrate that when considering geographical aspects and selection on resource use simultaneously, the lineages oscillate their degree of specialization throughout multiple speciation events, as predicted by the Oscillation Hypothesis. At the same time, stronger selective pressures and smaller dispersion capacity act simultaneously resulting in higher species richness. This study illustrates through different approaches how investigation on coevolutionary processes can help us better comprehend the dynamics of species coexistence and generation of biodiversity.

Keywords: Parasite-host. Ecological interactions. Coevolution. Speciation. Diversification.

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CAPÍTULO 1

INTRODUÇÃO GERAL: INTERAÇÕES RECÍPROCAS EM UM MUNDO EM CONSTANTE MUDANÇAS

Desde o aparecimento dos primeiros seres vivos no planeta Terra, a evolução e persistência das mais diversas formas de vida tem sido fortemente influenciada pela interação com outras espécies. Conceitos relacionados à dinâmica esperadas devido à interações recíprocas entre as espécies têm se tornado elementos chave no estudo de processos evolutivos. Em um clássico trabalho, Erlich & Raven (1964) foram os primeiros autores a sugerir que a grande diversidade de espécies de borboleta, um dos grupos de insetos mais diversos que existem (Mitter et al., 1988), poderia estar intimamente relacionada a uma adaptação ao uso de suas plantas hospedeiras. Ao estudar curvas de extinção de táxons, Van Valen (1973) percebeu que estas permaneciam constantes independentemente do grupo estudado. Esta observação o levou a propor a ideia de que espécies em determinada relação ecológica estão em uma perpétua “corrida armamentista”, no qual as espécies desenvolvem adaptações e contra-adaptações sem nunca chegarem a um equilíbrio. Ao longo das últimas décadas, diversos novos conceitos, modelos e experimentos foram desenvolvidos de modo a detalhar como interações recíprocas entre espécies afetam a sua evolução (Thompson, 1994). Tendo em vista o papel destas interações ecológicas em processos ecológicos e evolutivos, pode-se considerar a coevolução como um fenômeno essencial para se entender a organização da biodiversidade atual (Thompson, 1994; Thompson, 2005).

Em sua definição mais ampla, a coevolução pode ser definida como mudanças evolutivas recíprocas entre espécies que interagem e exercem pressões seletivas recíprocas entre si (Janzen, 1980). Entretanto, esta definição pode ser detalhada de acordo com a escala temporal e magnitude das mudanças causadas pela interação. Em especial, Brooks (1979) sugere que se utilize o termo co-acomodação para descrever adaptações em características das espécies envolvidas em interações recíprocas, sem que ocorra processos de especiação associados a esta interação. Por sua vez, o termo co-especiação descreve eventos em que a evolução da especificidade de uma espécie em relação à exploração da outra leva a formação de espécies distintas (Brooks, 1979; Brooks et al., 2015). Estas distinções se tornam importantes, uma vez que ressaltam que a interação entre espécies pode ter consequências tanto a um nível microevolutivo quanto macroevolutivo.

De acordo com a perspectiva adotada por Thompson (2005), podemos considerar que boa parte da evolução é de certa forma parte de um processo coevolutivo. A maior parte das espécies sobrevive e se reproduz com necessidade de uma outra espécie, seja de forma direta ou indireta. Espécies podem evoluir ao cooptar e manipular outras

espécies de vida livre, ou adquirir o genoma inteiro de outras espécies através de relação simbióticas como mutualismo e parasitismo (Thompson, 2005). Para fins de aplicações práticas para o interesse humano, fenômenos coevolutivos se aplicam para áreas de epidemiologia, aquicultura, agricultura, biologia da conservação, manejo florestal, entre tantos outros (Thompson, 2005).

Aqui, destaco duas áreas de interesse especial do entendimento de fenômenos coevolutivos: mudanças climáticas e o surgimento de doenças infecciosas emergentes (Brooks et al., 2019). Mudanças na biosfera através da alteração da paisagem, perturbações ecológicas e invasões de espécies podem ser amplamente atribuídas à atividade antropogênica (Hoberg & Brooks, 2015). Essas perturbações têm sido relacionadas a um aumento no número de doenças emergentes nas últimas décadas (Epstein et al., 2003). A introdução de espécies em novas regiões aumenta a possibilidade de mistura de organismos que nunca tiveram contato evolutivo prévio (Daszak et al., 2000). Um sistema de transporte integrado entre as diversas regiões do globo terrestre também favorece o surgimento de novas interações devido a mudanças na distribuição das espécies, o que pode levar à disseminação de patógenos que afetam a saúde das populações humanas, da vida selvagem e doméstica (Kilpatrick, 2011). Além disso, as mudanças climáticas alteram os padrões de movimento e a distribuição geográfica das espécies, juntamente com seus patógenos (Dobson & Carper, 1992; Daszak et al., 2000; Patz et al., 2008). Por fim, o contato de espécies previamente isoladas favorece o surgimento de doenças infecciosas, no que é denominado crise de doenças infecciosas emergentes (EID, do inglês *emerging infectious diseases*) (Brooks & Hoberg, 2006; Brooks & Hoberg, 2013).

O surgimento de doenças infecciosas pode apresentar grandes impactos à saúde, políticos e econômicos (Epstein et al., 2003; Newcomb et al., 2003). Eles também alteram o funcionamento do ecossistema e ameaçam a biodiversidade com maior risco de extinção para espécies vulneráveis (Harvell et al., 1999; Padersen et al., 2007). Desta forma, uma melhor compreensão da dinâmica coevolutiva como o de sistemas parasitas-hospedeiros pode nos ajudar a prever com mais precisão o que esperar durante períodos de mudanças climáticas e ambientais e permitir respostas mais eficientes para a prevenção ou mitigação dos impactos da EID (Agosta et al., 2010). Uma abordagem fundamental para compreender a EID é explorá-la como um fenômeno evolutivo e ecológico que ocorre como consequência do estabelecimento de novas interações de espécies anteriormente isoladas (Brooks & Hoberg, 2013). Por sua vez, o delineamento

de políticas e respostas apropriadas para estas questões necessitam de uma base teórica forte e bem embasada a respeito de processos coevolutivos.

Ao mesmo tempo em que se faz necessário um melhor entendimento de processos coevolutivos para a compreensão de fenômenos ecológicos e evolutivos, assim como para aplicações práticas de interesse humano, tem se percebido que muitos das visões tradicionais não se acomodam mais às evidências empíricas de como estes processos ocorrem na natureza. Um exemplo disso é o chamado “paradoxo do parasito”. O reconhecimento de que a maioria dos parasitas têm um número restrito de hospedeiros (Thompson 1994, 2005) levou à visão evolutiva tradicional a considerar os parasitas como especialistas em hospedeiros (Bernays, 1989; Agrawal, 2000; Bernays, 2001; Janz et al., 2005). Esse padrão de especialização levou à idéia de que a especialização é continuamente favorecida ao longo do tempo evolutivo, o que por sua vez leva as espécies a um “beco sem saída” evolutivo (Moran, 1988; Wiegmann et al., 1993; Kelley & Farrell, 1998). Por outro lado, vários estudos mostraram que linhagens generalistas de parasitas são derivadas de linhagens mais especializadas (Scheffer & Wiegmann, 2000; Janz et al., 2001, Yotoko et al., 2005). O “paradoxo do parasito”, portanto, descreve a contraditória ideia de que a especialização é sempre selecionada em parasitas com as grandes evidências mostrando eventos abundantes de troca de hospedeiro (Agosta et al., 2010). Ao se reconhecer que a especialização de parasitos é menos estrita do que esperado anteriormente, pode se compreender que um número diversificado de surtos de doenças infecciosas pode estar relacionado à dispersão de parasitas para novos hospedeiros que não tiveram tempo de desenvolver mecanismos de resistência (Brooks & Hoberg, 2013). Além disso, é também provável que essa troca de hospedeiro ocorra mesmo sem a evolução de novas capacidades de utilização do patógeno (Agosta & Klemens, 2008).

Nesse contexto, o Paradigma de Estocolmo foi proposto como um *framework* teórico que resolve os paradoxos derivados das visões tradicionais da teoria evolutiva relacionadas às associações interespecíficas (Hoberg & Brooks, 2015). Ele integra quatro conceitos básicos que explicam como as interações evoluem em diferentes escalas: *ecological fitting*, hipótese de oscilação e pulso de táxon (Hoberg & Brooks, 2015). O *ecological fitting* refere-se à capacidade do organismo de se adaptar rapidamente a novos hospedeiros devido a sua flexibilidade fenotípica e conservantismo filogenético, sem a necessidade de novidades evolutivas para que ocorra a troca de hospedeiros (Agosta & Klemens, 2008). Essa flexibilidade pode resultar em oscilações

no número de hospedeiros usados por um organismo, com especialistas dando origem a generalistas, e generalistas se adaptando e diversificando em especialistas, conforme previsto pela Hipótese de Oscilação (Janz & Nylin, 2008; Nylin et al., 2014). A Teoria do Mosaico Geográfico da Coevolução incorpora os efeitos da distribuição espacial heterogênea das diferentes espécies nas dinâmicas coevolutivas (Thompson, 2005). Finalmente, a história das mudanças adaptativas ao longo do espaço e tempo geográficos de uma linhagem resulta no Pulso de Táxons (Erwin, 1985).

O Paradigma de Estocolmo é consistente com o conceito de vida como um sistema complexo. Uma característica chave que é inerente a qualquer sistema complexo é a propriedade de emergência, na qual comportamentos surgem da interação de seus componentes de nível inferior e não podem ser detectados por um estudo isolado de suas partes (Bar-Yam, 1997). Desta forma, mecanismos que operam em interações ecológicas em níveis de escala mais baixos, como o *ecological fitting*, podem resultar nas dinâmicas emergentes observadas em níveis de organização mais altos, como a oscilação do uso de hospedeiros ao longo de linhagens evolutivas.

Devido à complexidade dos fenômenos coevolutivos e às longas escalas temporais envolvidas, avanços substanciais no entendimento destes fenômenos podem ser alcançados pelo uso de modelos matemáticos e computacionais (Smith & Slaktin, 1979; Abrams, 2000; Bergelson et al., 2001). Em especial, modelos matemáticos podem servir para avaliar a validade do encadeamento lógico de modelos verbais em uma abordagem conhecida como “modelos de prova de conceito” (Servedio et al., 2014). Estes modelos traduzem pressupostos verbais em princípios matemáticos, e então é feita a comparação das previsões derivadas dos modelos verbais com a gerada pelos modelos matemáticos. Nos artigos apresentados nesta tese, são investigados dois problemas teóricos a respeito de fenômenos coevolutivos utilizando-se análises por modelagem computacional.

No segundo capítulo, estudamos a dinâmica coevolutiva entre um par de espécies que interagem de forma antagonista ao comparar dois tipos de modos reprodutivos: sexuada e assexuada. Embora a reprodução sexuada seja uma estratégia reprodutiva bastante prevalente nos organismos (Michod & Levin, 1988), existe um amplo debate a respeito de quais mecanismos evolutivos favorecem o seu surgimento e permanência na natureza (Smith, 1971; Otto & Lenormand, 2002). A partir deste debate, foi proposta a hipótese de que interações entre parasitos e hospedeiros podem ter um papel fundamental para explicar a vantagem da reprodução sexuada em relação à assexuada

(Jaenike, 1978; Bremermann, 1980; Hamilton, 1980). Embora muitos desses estudos abordem quais condições favorecem cada uma dessas estratégias, o impacto dessas estratégias reprodutivas na dinâmica coevolutiva de interações parasito-hospedeiro ainda é pouco compreendido. Desta forma, neste capítulo investigamos como a forma de reprodução influencia a evolução de fenótipos de duas espécies em resposta à interação antagonista entre elas. Dado que a resposta evolutiva à interação se dá a partir dos fenótipos da espécie exploradora e da vítima, a forma no qual essas características são herdadas pelos descendentes pode influenciar o resultado da dinâmica ao longo das gerações. Em especial, estudamos as dinâmicas esperadas para interações determinadas por fenótipos quantitativos em indivíduos com genoma explicitamente modelado. Para isso, usamos um modelo baseada em indivíduos, no qual a aptidão se dá pelo ajuste fenotípico dos indivíduos e a intensidade de interação tanto para o explorador quanto para a vítima. Nossos resultados demonstram que a dinâmica coevolutiva resultante é bastante dependente da estratégia reprodutiva utilizada pelas espécies. Ao passo em que no modelo de reprodução sexuada resultam em dinâmicas centralizadas ou oscilatórias, nos modelos de reprodução assexuada as dinâmicas resultam em bifurcações do fenótipo seguidas ou não de extinção da espécie exploradora. Este último processo sugere que fenômenos de bifurcação do fenótipo podem ser menos comuns do que esperado anteriormente em outros tipos de interações ecológicas (Doebeli & Dieckman, 2000). Em contextos evolutivos de interações antagonistas mediadas por caracteres quantitativos, a estratégia sexuada também apresentar maior probabilidade de persistência em comparação à estratégia de reprodução assexuada. Por fim, considerando quão comum a reprodução sexuada ocorre na natureza, a conclusão de modelos coevolutivos que estudem a evolução de fenótipos devido à interação de espécies pode ser fortemente influenciada pela escolha da estratégia de reprodução assumida dentro de seus pressupostos.

No terceiro capítulo, é investigado como o espaço geográfico interage com a pressão seletiva de diferentes hospedeiros e influenciam o processo de diversificação e evolução do tamanho do repertório de espécies em linhagens. Este processo se refere às consequências macroevolutivas de interações coevolutivas, e busca oferecer contribuições para o entendimento do papel da coevolução na diversificação das espécies. Em particular, damos continuidade à abordagem desenvolvida por Braga et al., (2018) em um modelo espacialmente explícito, de modo a avaliar previsões teóricas da Hipótese da Oscilação (Janz & Nylin, 2008). Neste trabalho, a reprodução sexuada e

o uso de um genoma modelado explicitamente são elementos fundamentais do modelo, pois permitem avaliar a evolução das linhagens em termos do surgimento de diferentes espécies, caracterizadas pelo critério de grupos de indivíduos reprodutivamente isolados devido à incompatibilidade genotípica. Utilizando um modelo baseado em indivíduos, estudamos a variação do repertório do hospedeiro ao longo de múltiplos eventos de especiação para cenários no qual os indivíduos estão sujeitos à diferentes intensidades de pressão seletiva e possuem diferentes capacidades de dispersão no espaço. Ao medirmos a proporção de eventos de expansão do número de hospedeiros seguido por eventos de especialização, encontramos que oscilações no tamanho do repertório de hospedeiros ocorreram em todos os cenários avaliados. Além disso, os efeitos do aumento da intensidade da seleção e diminuição da capacidade de dispersão atuaram de forma conjunta de modo a resultar em uma maior riqueza de espécies. As variações no tamanho do repertório do hospedeiro são congruentes com as expectativas teóricas da Hipótese da Oscilação (Janz & Nylin, 2008): linhagens experimentam ao longo de sua história evolutiva diferentes fases de expansão do tamanho de seu repertório de hospedeiros, seguidos de redução do tamanho desse repertório (especialização). Desta forma, a diversificação de espécies que utilizam outro grupo de espécies como recurso é acompanhada por oscilações no uso de seus hospedeiros, e não por especialização contínua (Agosta et al., 2010). A demonstração da Hipótese da Oscilação em um modelo espacialmente explícito mostra como tanto o espaço quanto interações entre espécies são fatores importantes para a compreensão de padrões de formação da biodiversidade e evolução do grau de especialização das linhagens, atuando de forma não-exclusiva.

Nesta tese, busquei investigar como interações antagonistas apresentam consequências para a evolução das espécies em diferentes escalas de tempo. Em uma escala microevolutiva, demonstramos que tanto a persistência da interação quanto a evolução dos fenótipos são fortemente influenciados pela estratégia reprodutiva das espécies avaliadas. Em uma escala macroevolutiva, as pressões seletivas dadas pela interação ecológica junto com aspectos geográficos interagem de modo a influenciar a riqueza de espécies, e oscilações no tamanho do repertório de hospedeiros emergem ao longo desta dinâmica, conforme previsto pela Hipótese da Oscilação. De forma conjunta, estes dois trabalhos expandem o nosso conhecimento a respeito das consequências evolutivas de interações antagonistas, fundamentais para o entendimento das mudanças globais que a humanidade enfrenta neste momento atual (Hoberg & Brooks, 2015).

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CAPÍTULO 2

THE INFLUENCE OF REPRODUCTIVE STRATEGY IN THE COEVOLUTIONARY DYNAMICS OF ANTAGONISTIC INTERACTION

The Influence of Reproductive Strategy in the Coevolutionary Dynamics of Antagonistic Interaction

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ABSTRACT

The conflict in antagonistic species produces dynamics in which adaptations and counter-adaptations evolve continuously and result in different evolutionary scenarios. However, predictions on the outcomes of these dynamics can be largely influenced by the underpinning genetic details of the interaction, which in turn can be different for sexual and asexual reproduction modes. The objective of this paper was to investigate how the selection caused by the antagonistic interaction between two species influences the evolution of their phenotypes. Using individual-based simulations, each individual was characterized by their trophic level (exploiter or victim) and explicit genome composed of multiple loci that resulted in a quantitative trait. The interaction of individuals from each population resulted in fitness (probability of survival) as a function of the phenotypic difference between exploiter and victim and the intensity of the interaction pressure for each species. Surviving individuals reproduced, leaving offspring for the next generation. We compared the coevolutionary dynamics of sexual and asexual reproductive strategies. The simulations varied in different combinations of interaction pressure. For sexual reproduction, we observed that the phenotypes evolved in either centralized or oscillatory patterns. The asexual reproduction model resulted in the appearance of evolutionary branching and extinction of the exploiter population. Our simulations demonstrate that assumptions on sexual and asexual reproduction modes can have important consequences on determining the evolutionary dynamics of the interaction. We conclude that considering how genetic information and phenotypic traits are transmitted between generations has great relevance when studying the evolutionary dynamics of interacting species.

Keywords: Coevolution. Antagonistic interaction. Reproductive strategy.

1 INTRODUCTION

Despite the ubiquity of sexual reproduction in nature (Michod & Levin, 1988), its persistence has long intrigued evolutionary biologists in what is defined as the “paradox of sex” (Otto & Lenormand, 2002). Compared to asexual reproduction, there are substantial disadvantages associated with this reproductive strategy (De Visser & Elena, 2007). For instance, females that reproduce asexually can produce double the offspring when compared to a sexual counterpart (Smith, 1971). Investing in sexual reproduction is also energetically costly in terms of finding individuals from the opposite sex (Smith, 1978) and it is associated with subsidiary costs in the production of reproductive structures (Solbrig, 1976). In order to account for its widespread use in nature, advantages of sexual reproduction should outweigh its disadvantages (Barton, 1998). One of the most prominent hypotheses to explain the persistence of sex proposes that the coevolutionary arms-race between parasites and hosts can play a key role in the evolution of sexual reproduction (Jaenike, 1978; Bremermann, 1980; Hamilton, 1980). This debate was followed by numerous studies and the development of theoretical models to understand the contribution of biotic interactions for explaining the evolutionary significance of sex (Barton & Charlesworth, 1998; West et al., 1999; Otto & Lenormand, 2002; Koskella & Lively, 2009).

The main argument for the role of parasites on the evolution of sexual reproduction stands on the idea that sex promotes adaptation to fluctuating environments, as it produces more genetic variability than asexual reproduction (Burt, 2000; Otto & Barton, 2001). In turn, coevolving parasites act as the main driving force that represents this changing environment (Bel et al., 1987; Seger & Hamilton, 1988; Hamilton & Axelrod, 1990). Despite the popularity of this idea, an increasing body of theoretical models suggests that the scenarios where this hypothesis applies are more strict than previously thought (Kondrashov, 1993; Otto & Feldman, 1997; Otto & Lenormand, 2002), reinforcing that embracing complex features of natural systems is essential for a better understanding of the relationship between parasite-host interactions and sex (Otto & Lenormand, 2002).

Typically, the genetic models that are used to investigate the performance of sexual and asexual reproduction modes and the effects of recombination incorporate only one or a few loci (Barton, 1995; Howard & Lively, 1998; Peters & Lively, 1999). The same approach has been applied to understand the coevolutionary dynamics in parasite-host

interactions (Gavrilets & Hastings, 1998; Bell & Smith, 1987; Seger 1988; Preigel & Korol, 1990; Kirzhner et al., 1999). Other models disregard or simplify the genetic basis and assume that coevolution is mediated by phenotypic interactions. The description of these dynamics has already been studied by the use of adaptive dynamics (Abrams 2001; Dieckmann & Law, 1996; Doebeli & Dieckmann, 2000; Dercole et al., 2003), game theory (Brown & Vincent, 1992), or quantitative genetics (Saloniemi, 1993; Abrams & Matsuda, 1997; Gavrilets, 1997; Khibnik & Kondrashov, 1997). These models made critical contributions to the development of the theoretical foundations on the field of evolutionary biology. Nevertheless, it has also been shown that the details of the genetic basis and the expressed phenotypic traits can have important consequences for the predicted outcomes of evolutionary models (Nagylaki, 1991; Bürger, 2000, Gavrilets & Hastings, 1995; Bürger, 2002a; Bürger, 2002b; Bürger, 2005).

Traits that are determined by the interaction of multiple loci or that assume quantitative values result in evolutionary dynamics that cannot be inferred by simpler models (Kopp & Gavrilets, 2006). At the same time, a range of coevolutionary interactions is mediated by quantitative traits, with important implications on the coevolutionary process (Thompson, 1999). Some examples include continuous morphological traits such as claw strength and shell thickness in crabs and gastropods (West et al., 1991) and bill morphologies of North American crossbills and pinecone sizes (Benkman, 1999). Brood nest parasites are favored by increasing the similarity of their eggs when compared to their hosts, avoiding nest rejection (Soler et al., 2001). The concentration of defensive compounds in plants and the activity of detoxifying enzymes in insects determine the plant susceptibility to the attack of herbivores (Berenbaum et al., 1986; Berenbaum & Zangerl 1998; Bergelson et al., 2001). Quantitative variation in traits closely related to coevolutionary dynamics has also been reported for aphids and parasitoid wasps (Henter 1995; Henter & Via, 1995), newts and snakes (Brodie & Brodie, 1999), prey and predators (Benkman, 1999; Abrams 2000; Brodie et al., 2002), and pollinators and plants (Schemske & Horvitz, 1989; Steiner & Whitehead, 1991; O'Neil, 1999; Galen & Cuba, 2001; Alexandersson & Johnson, 2002).

So far, the few models that investigated the coevolutionary dynamics of parasite-host interactions mediated by quantitative traits assumed either asexual (Frank, 1994) or sexual reproduction (Nuismer & Doebeli, 2004, Nuismer et al., 2005; Nuismer et al., 2007). However, a direct comparison of the effects of reproductive modes for parasite-host interactions determined by quantitative traits indicates that sexual and asexual

species yield distinct effects on populational dynamics and phenotypic variability (Doebeli, 1996a). Furthermore, on a wide variety of other ecological interactions that incorporate explicit genetic models, assumptions on species reproductive strategy had strong implications for the evolutionary results of these interactions (Doebeli & Dieckmann, 2000). In particular, asexual reproduction and assortative mating can result in evolutionary branching, while sexual reproduction with random mating precludes the emergence of this pattern (Doebeli & Dieckmann, 2000). Despite the potential implications of the reproductive strategy on the coevolutionary dynamics of antagonistic interactions, theoretical predictions about the effects of sexual and asexual reproduction remain largely unexplored.

In this paper, we address this gap by investigating the effects of reproductive strategy on antagonistic interactions that are mediated by quantitative traits on genetic explicit models. We used individual-based simulations to investigate the evolutionary dynamics of two species with antagonistic interaction subject to sexual and asexual strategies of reproduction. The term “antagonist” is used to refer generally to any trophic interaction where one species benefits from the interaction at the expense of the other, such as parasite-host, parasitoid-host or phytophagous-plant interactions. As existing models suggest that explicit multilocus genetics can significantly alter predictions on the evolutionary dynamics (Doebeli, 1996; Kopp & Gavrillets, 2006), we developed an explicit genetic model composed by multiple loci where the phenotype is composed by the additive effect of each locus. Fitness effects of the interaction are mediated by quantitative traits and the effectivity of the interaction is set by trait matching. The interaction pressure measures how the fitness of one individual is affected by the interaction and is distinct for each species. We compared the outcomes for asexual and sexual reproductive strategies on the patterns of phenotypic evolution for both species. We demonstrate that the coevolutionary dynamics on antagonistic interactions are influenced by the reproductive strategy and that explicitly modeling the genetic information of individuals results in dynamics that were not predicted by analytical models.

2 MATERIAL AND METHODS

2.1 MODEL DESCRIPTION

We simulated the coevolutionary dynamics between two species that interact antagonistically using individual-based modeling (IBM). The model is based on the concepts of coevolutionary dynamics, in which selective pressures between species with antagonistic interactions influence reciprocally the phenotype and genotype of each interacting species (de Vienne et al., 2012). The explicit modeling of the genome is based on the framework used by Aguiar et al., (2009) and Nagai et al., (2016). We adopt in this model a selection based on trait matching, as already reported for parasite-host systems (Benkman 1999; Clayton et al., 2003; Soler et al., 2001). We compared the effect of reproductive strategies and the intensity of interaction pressure due to the intensity of the interaction. The description of the model is based on the ODD protocol to describe aspects of individual-based modeling (Grimm et al., 2006; Grimm et al., 2010). The design concepts are described in Supplementary Material 1.

The model consists of two populations from distinct trophic levels that interact antagonistically: an exploiter species E_i and a victim species V_j , where the subscripts identify each population individual, respectively. The number of individuals in a population is K , which represents the carrying capacity of each population. The term exploiter may refer to any species that exploit other species in order to feed itself or complete its life cycle while potentially causing injuries in this process, and can include examples like phytophagous insects, parasites and parasitoids. The term victim may refer to any species that is ecologically exploited by others and can encompass plants and hosts. For simplicity, the individuals are modeled as haploids and hermaphrodites. Their genome consists of strings of size L with binary loci. The phenotypes are determined by the sum of all values of the string:

$$p_i = \sum_{l=1}^L X_{i,l}$$

where $X_{i,l} \in \{0,1\}$. All possible phenotype values range from $0 \leq p_i \leq L$. A population is composed of all individuals of each trophic level at a given generation t , and it is characterized by the frequency distribution of the phenotype of all individuals.

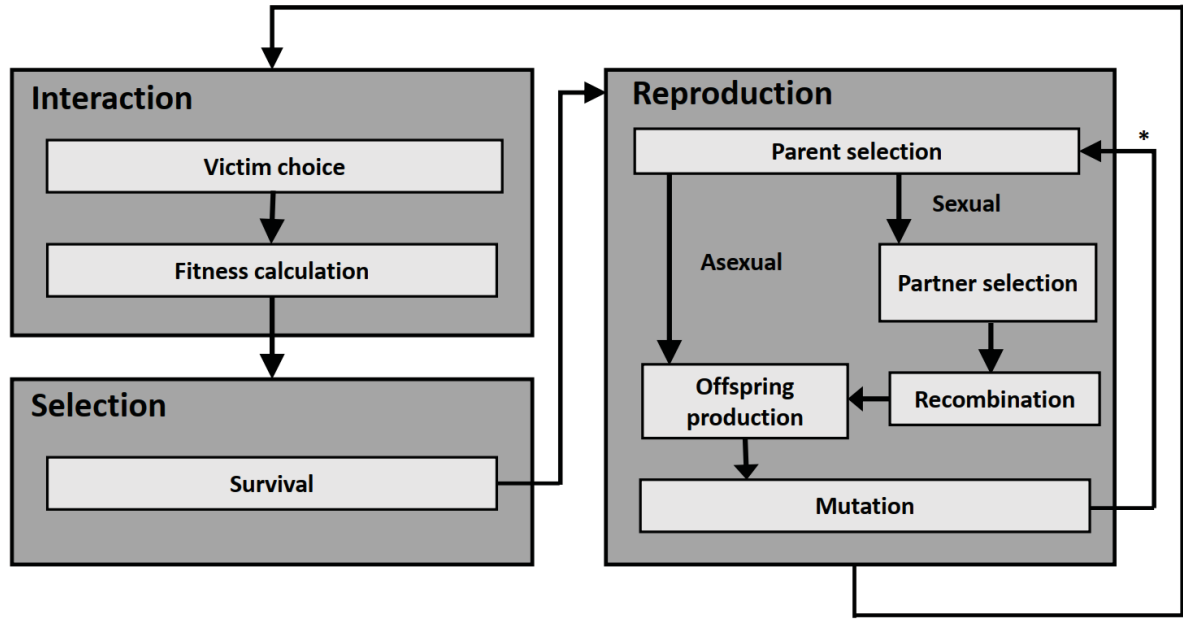


Figure 1. Fluxogram of scheduling process of the model. * Indicates that the process is repeated until the carrying capacity is reached.

Each time step represents one generation for both exploiter and victim populations. Within each generation, three phases occur in the following order: interaction, selection, and reproduction (Fig. 1). In the interaction phase, the first step (victim choice) allows each exploiter i to interact with a randomly assigned victim j . Fitness calculation assumes that the interaction between the antagonistic species exerts selective pressures according to the trait matching between individuals. Fitness determines the survival probability for each individual. Exploiter's fitness W_i^e is given by:

$$W_i^e = \exp \left[-\alpha (e_i - v_j)^2 \right],$$

where α represents the intensity of the interaction pressure on the exploiter, e_i the phenotype value of exploiter i , and v_j the phenotype of the victim j . Thus, the exploiter will have maximum fitness when its phenotype is equal to the victim's phenotype, and its fitness will decrease the more distant its phenotype is in relation to the chosen victim (Fig. 2A).

The victim's fitness is calculated after all interaction occurs, as a function of the sum of all attacks to each individual:

$$W_j^v = \exp \left[-\beta \left(\sum_{\{i \rightarrow j\}} W_i^e \right)^2 \right]$$

where β is the strength of the interaction pressure on the victim species and $\sum_{\{i \rightarrow j\}} W_i^e$ is the sum of the fitnesses of all the exploiters that interact with the victim j at this generation. The victim will have a maximum fitness if it was not attacked, and its fitness will decrease according to the number of interactions and the strength of attacks (W_i^e) on the victim (Fig. 2B).

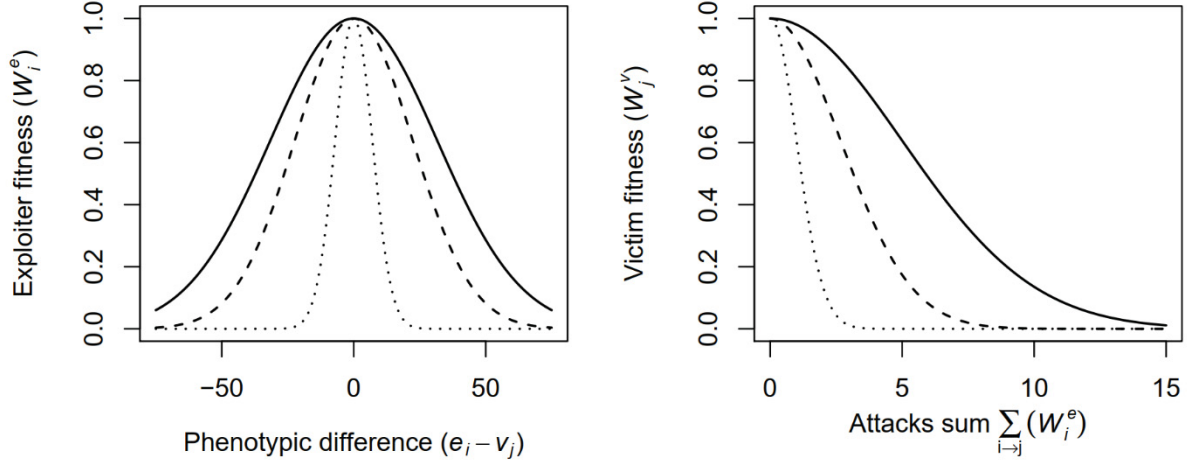


Figure 2. A: Relationship between exploiter fitness (W_i^e) and phenotypic difference between exploiter and victim as a function of different intensities of interaction pressure for the exploiter (α). Solid line: $\alpha = 0.0005$; Dashed line: $\alpha = 0.001$; Dotted line: $\alpha = 0.01$. B. Relationship between the victim fitness (W_j^v) and sum of attacks from the exploiter as a function of different intensities of interaction pressure on the victim (β). Solid line: $\beta = 0.02$; Dashed line: $\beta = 0.07$; Dotted line: $\beta = 0.5$.

At the selection phase, individuals from each population survive according to the probability given by its fitness value. Those who survive remain in the population and participate in reproduction for the next phase of the model. If no individual survives at this phase, we consider that the population is extinct and the simulation ends. The same applies if only one individual survives in the model with sexual reproductive strategy (see below), as a pair of individuals is necessary to generate new offspring.

We compared two reproductive strategies: both trophic levels assume either asexual reproduction or sexual reproduction. Regardless of the strategy, an individual is chosen randomly from the population to reproduce (parent selection). The following steps depend on the reproductive strategy. In the asexual reproduction model, the genome inherited by the offspring is equal to its parent's genome. For the model with sexual reproduction, a partner is chosen with equal probability among all individuals in the population and the offspring's genome inherits each parent's loci with a 50% chance. Finally, each locus of the offspring has a probability of mutating as specified by a mutation

rate μ . The reproductive process is repeated until the carrying capacity is reached. We note that this assumption implies that one individual (in the asexual reproduction model) or a pair of individuals (in the sexual reproduction model) are capable of recomposing the whole population on the next generation, in case they represent the only survivors after the interaction. After reproduction, a new generation starts and the cycle restarts.

Table 1. List of parameters used in the model with explicit genome modeling. Underlined values indicate the ones used in the main text.

Description	Parameter	Value
Carrying capacity	K	500, <u>1500</u>
Genome size	L	25, 50, <u>150</u> , 500, 1500
Total number of generations	N_{gen}	<u>5000</u>
Mutation rate per locus	μ	0.001, <u>0.0001</u>
Intensity of the interaction pressure on the exploiter	α	<u>0.01, 0.05, 0.1, 0.5, 1.0, 5.0</u>
Intensity of the interaction pressure on the victim	β	<u>0.01, 0.05, 0.1, 0.5, 1.0, 5.0</u>

2.2 ANALYSIS OF THE RESULTS AND ROBUSTNESS

We investigated the coevolutionary phenotype dynamics for combinations of the intensity of interaction pressure on exploiter and victim (α and β , see table 1). The coevolutionary dynamics were described by the pattern of phenotype distribution of both exploiter and victim through generations. The initial condition of every model considered that the population size of both exploiters and victims were equal to their carrying capacity, and the phenotype value of each individual was equal to half of the genome size. For each combination of parameters, we repeated the simulation 10 times. For the same parameter combination, we also recorded the number of simulations that resulted in extinction and the number of generations until extinction occurred.

To access the robustness of our results, we also tested different combinations of other parameters of the model: genome size, carrying capacity, and mutation rate. To evaluate the assumption of explicitly modeling the genome influenced the dynamics, we

built an equivalent version of the model which considered the phenotypes as continuous traits and measured as a real finite number. In this version, the binary string that characterized the genome was not included. In order to maintain the phenotype values within a finite range we included an external stabilizing pressure (Gavrilets, 1997), that acts as a selective pressure towards an optimum favored phenotype:

$$W_i^{ext} = \exp[-\gamma (p_i - \theta_{otm})^2],$$

where, γ is the intensity of the external stabilizing pressure, p_i is the phenotype of the exploiter or victim, θ_{otm} is the optimum phenotype imposed by the stabilizing pressure, and W_i^{ext} is the effect of the stabilizing pressure on the fitness of the individual. The final fitness of the individual i (W_i^{final}) is given by:

$$W_i^{final} = W_i^{int} * W_i^{ext},$$

where W_i^{int} is the fitness given by the interaction and W_i^{ext} is the fitness given by the external stabilizing pressure. On the asexual reproduction mode, the offsprings inherit a phenotype value equal to its parent plus a variation ρ , a random number that follows a normal distribution according to:

$$P(\rho) = \frac{1}{\delta\sqrt{2\pi}} \exp\left(-\frac{\rho^2}{2\delta^2}\right)$$

where $P(\rho)$ is the probability of a variation of value ρ and standard deviation δ . To simulate the effects of sexual reproduction, we considered that the phenotype of the offspring was equal to the mean value between both parents' phenotypes, plus the variation ρ .

3 RESULTS

3.1 COEVOLUTIONARY DYNAMICS

The coevolutionary dynamics for the scenarios with sexual reproduction resulted in two different qualitative patterns of phenotype evolution through generations: central and oscillatory patterns. For the central pattern, the mean phenotype values of both species remained close to each other and showed small variation through generations (Fig. 3A). The phenotypic variance of the exploiter remained smaller than the variance of the victim, as the exploiters benefit from the most frequent victim phenotypes. In the oscillatory pattern, the mean phenotype value of the victim population oscillated along with the generations, as the exploiter population exerted a strong negative selection on the most frequent phenotypes of the victim population (Fig. 3B). This selective pressure on the most abundant phenotypes resulted in a shift of the mean phenotype value in the victim, followed by a change in the mean phenotype value of the exploiter. The distribution of phenotypes of both species oscillated through generations without reaching equilibrium.

The coevolutionary dynamics for sexual reproduction was sensitive to the selection strength of exploiters and victims. A low intensity of interaction pressure on the victim resulted in the central pattern, as the victim's phenotype distribution had small variation through generations (Fig. 4, upper panels). Increasing the strength of interaction pressure on the exploiter did not change the centralized pattern, but it resulted in a smaller variance in the exploiter's phenotype distribution. However, an increase in the interaction pressure on the victim shifted the dynamics to the oscillatory pattern (Fig. 4, middle and lower panels). The direction of the oscillations was not regular, and the amplitude of oscillations was higher when the intensity of interaction pressure on both victim and exploiter was high. The interactions coexisted in every combination of parameters of alpha and beta, with no extinction of the populations.

In the asexual scenario, the evolutionary dynamics were characterized either by the central pattern or by the appearance of evolutionary branching. In the latter pattern, the interaction pressure on the victim initially affected with greater intensity the intermediary values of the victim phenotype, decreasing its abundance while favoring phenotype values on the extremes of the distribution. This disruptive selection eventually produced two separate branches on the victim phenotype distribution. The frequency of

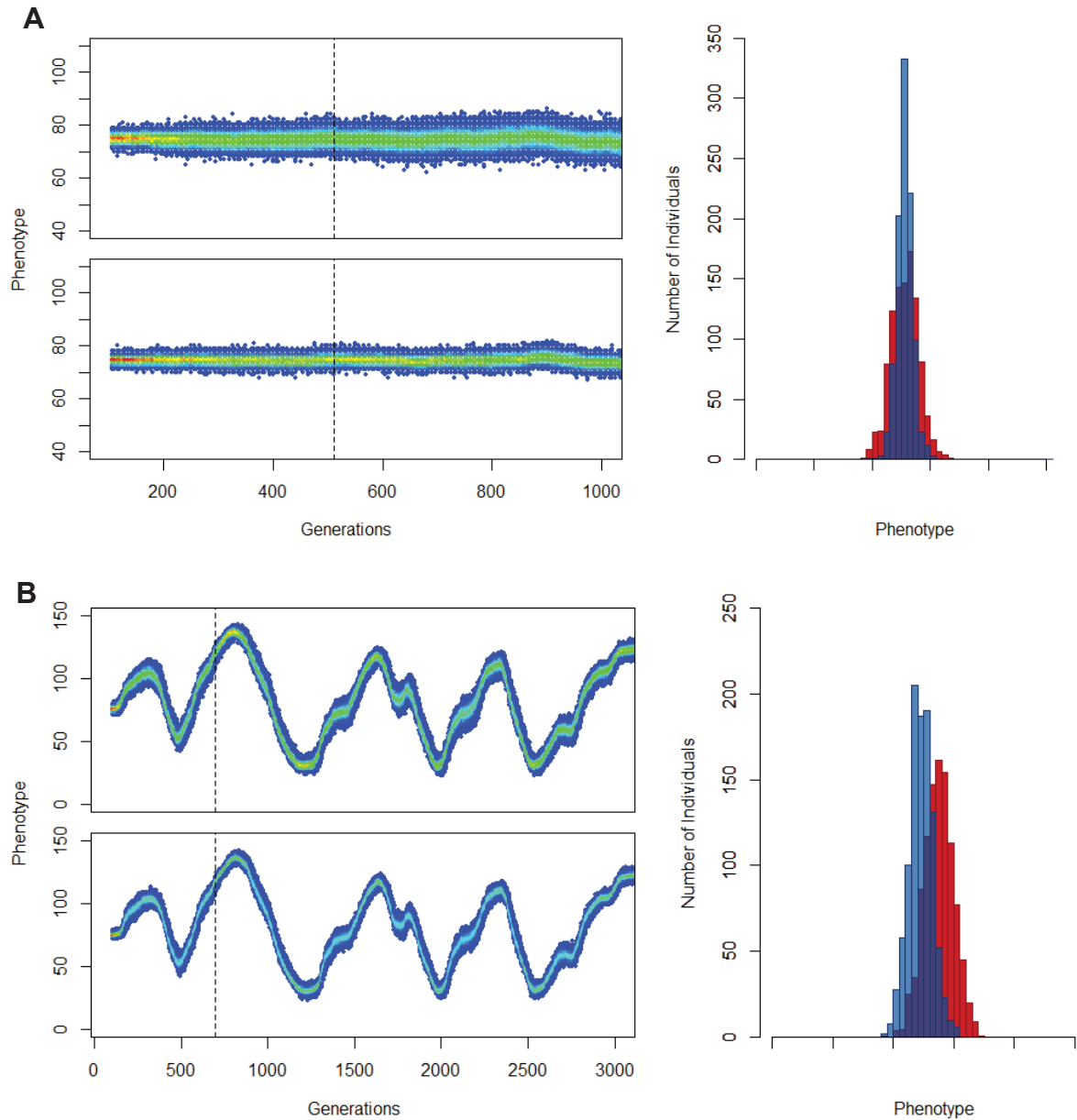


Figure 3. Coevolutionary dynamics between exploiter and victim population phenotypes. A: Central pattern; B: Oscillatory pattern. Left panels depict the phenotype evolution along with the generations for the victim (above) and the exploiter (below). The panel on the right shows the frequency of individuals with each phenotype at one particular generation, indicated by the dashed line at the left panel. On the left panels, colors indicate the frequency of individuals according to their phenotype, ranging from blue (small frequency of individuals) to green and red (highest frequency of individuals). On the right panel, exploiters are represented in red, while victims are represented in blue. Parameters were: $K = 1500$, $L = 150$, $\mu = 0.0001$. A: $\alpha = 0.01$, $\beta = 0.01$; B: $\alpha = 0.1$, $\beta = 5.0$.

individuals in each branch was strongly affected by the exploiters' interaction pressure. When one of the branches increased its number of individuals, the exploiters with phenotype close to this branch were favored and the phenotype distribution started to move closer to it. This led to a decrease in the number of exploiters on this branch while increasing the frequency of exploiters on the other. In turn, exploiters on the other branch

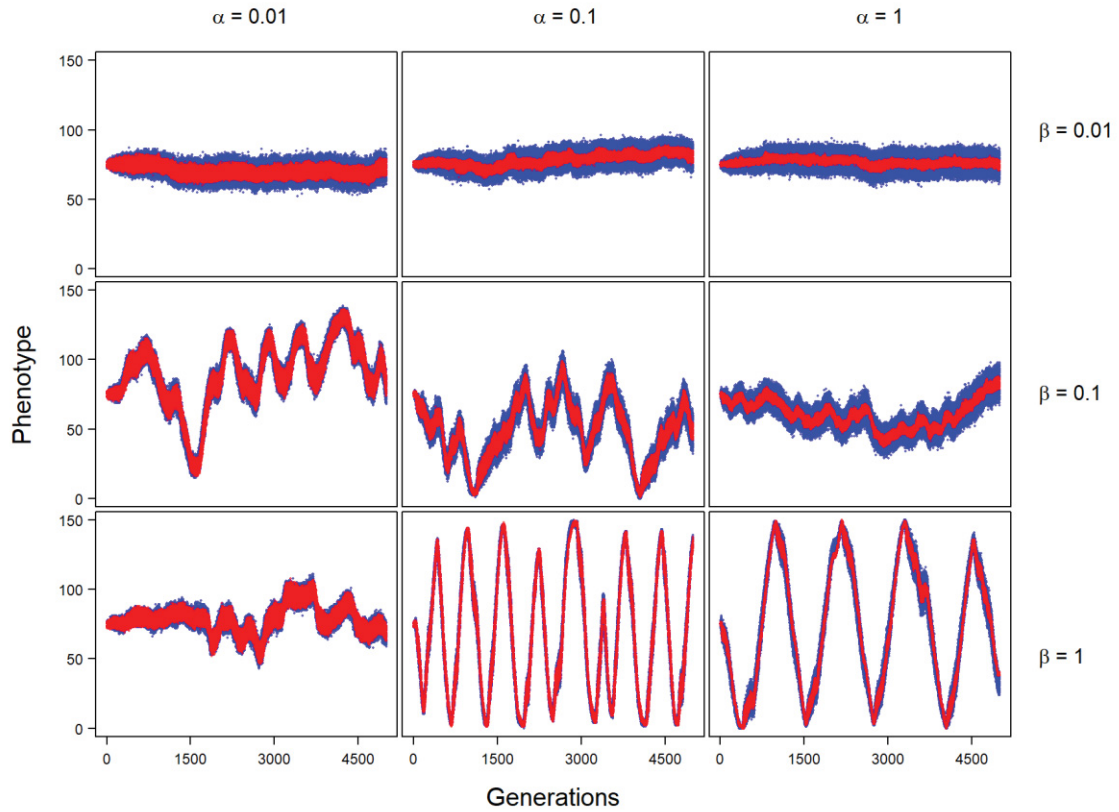


Figure 4. Coevolutionary dynamics for the exploiter (red) and victim (blue) along with generations for the model with sexual reproduction. Increasing the intensity of the interaction pressure for the exploiter (alpha) and victim (beta) leads to oscillation in the phenotypic dynamics resulting from the interaction. Parameters were: $K = 1500$, $L = 150$, $\mu = 0.0001$, $N_{gen} = 5000$.

started to increase their number and favored exploiters phenotype closer to them. Consequently, the mean phenotype distribution of the exploiter stayed either close to an intermediary position between both branches or oscillating between them. The bifurcations were not stable, as eventually one of the branches extinguished due to the selective pressure. After that, the exploiter phenotype distribution returned to the center of the remaining lineage and the process restarted (Fig. 5A). In most scenarios, eventually the exploiter was not able to successfully use the other branch as one of them was extinguished, leading to the extinction of the parasite population and the end of the interaction (Fig. 5B). We had no cases where the interaction led the victim population to be extinct. This can be explained as victims are randomly chosen by the exploiter, and more than one victim can choose the same victim. Thus, it is very unlikely that all victims are chosen and do not survive in the same generation, even if the interaction pressure is high.

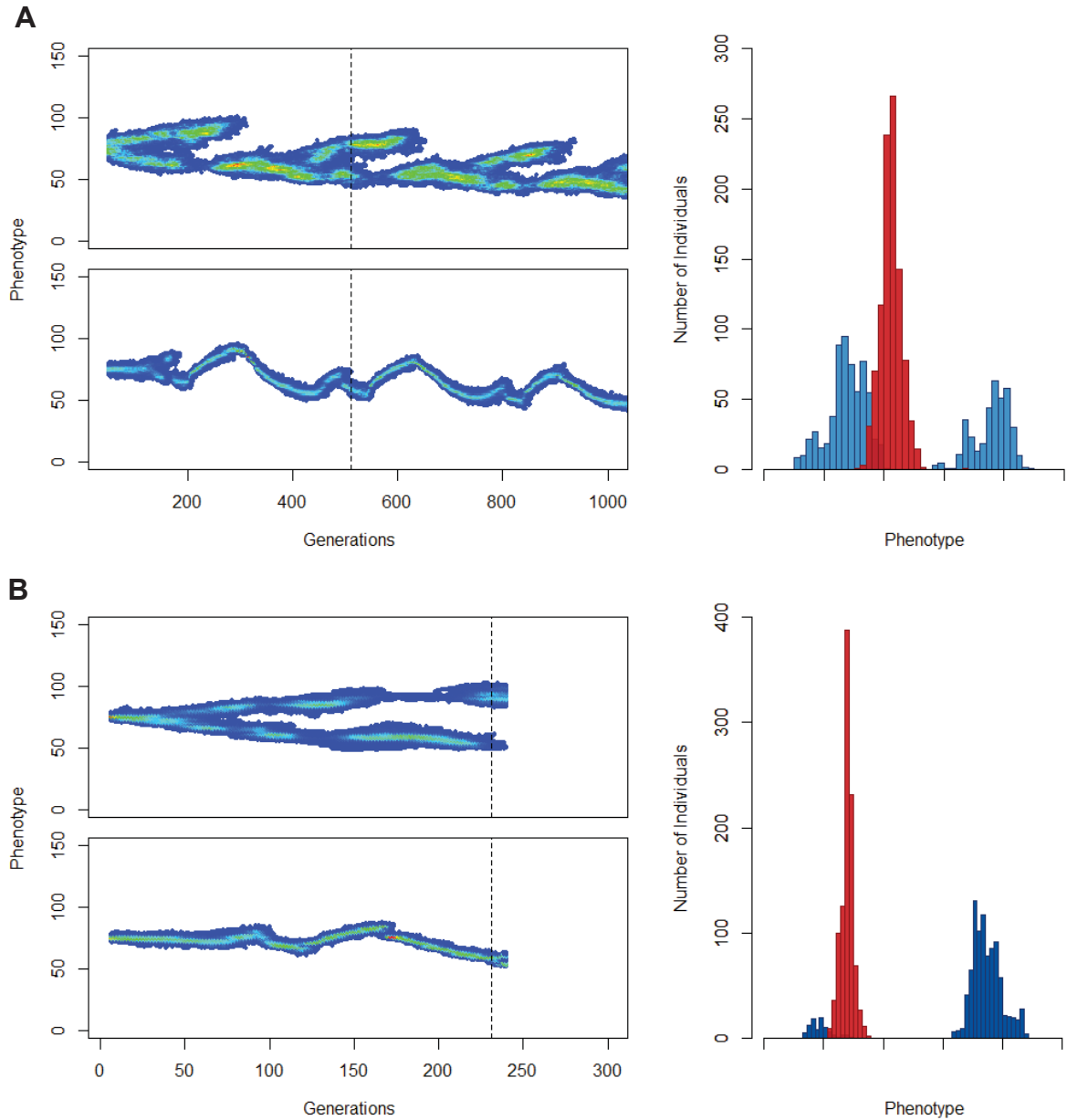


Figure 5. Coevolutionary outcomes for the antagonistic dynamics when individuals reproduce asexually. A) Evolutionary branching. B) Evolutionary branching followed by extinction. The left panel depicts the phenotype evolution along with the generations for the victim (above) and the exploiter (below). The right panel shows the frequency of individuals with each phenotype for both exploiter and victim populations at one particular generation (dotted line at the left panels). On the right panels, colors indicate the frequency of individuals according to their phenotype, ranging from blue (small frequency of individuals) to green and red (highest frequency of individuals). On the left panel, exploiters are represented in red, while victims are represented in blue. A: $\alpha = 0.01$, $\beta = 0.1$; B: $\alpha = 0.01$, $\beta = 0.5$.

The persistence or extinction of the interaction was strongly dependent on the strength of interaction pressure (Fig. 6A). For the low intensity of interaction pressure on the victim, the selective pressure exerted by the exploiter did not cause evolutionary branching and the interaction persisted. However, a more intense interaction pressure on the victim caused the formation of evolutionary branching, which in turn resulted in the eventual

extinction of the exploiter population. The number of generations until the extinction occurred was strongly related to the interaction pressure on exploiter and victim (Fig. 6B). A low interaction pressure on the exploiter or the victim allowed the interaction to persist for many generations until the exploiter went extinct. On the other side, a more intense interaction pressure on either species led to the extinction of the interaction in a shorter number of generations.

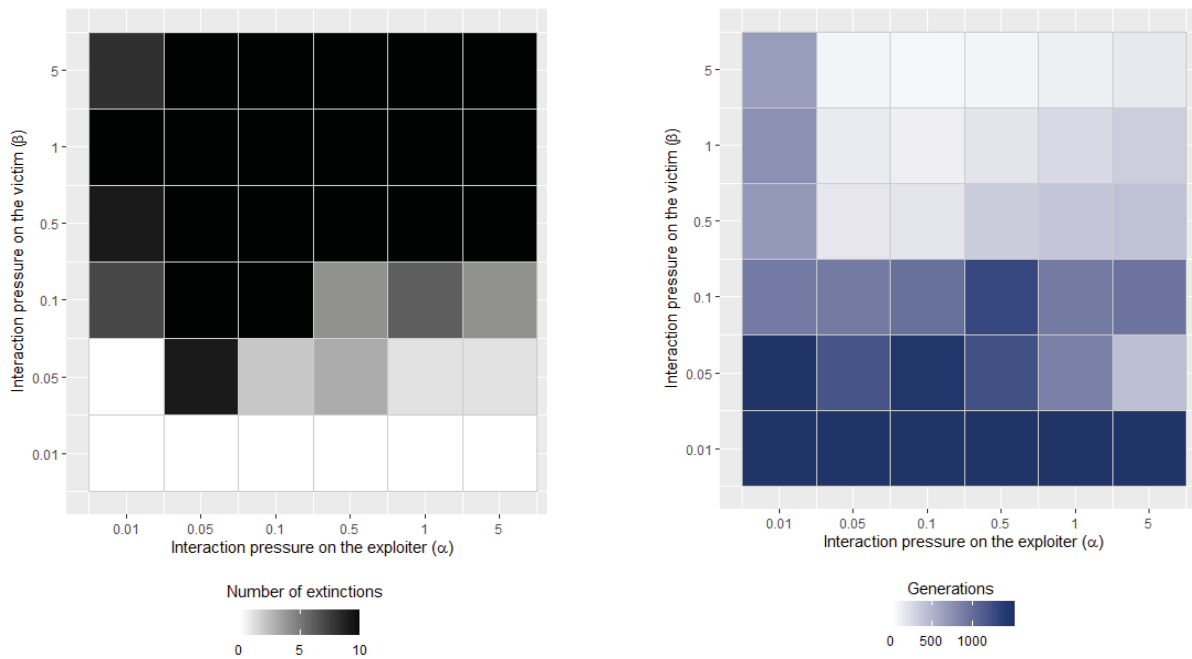


Figure 6. Frequency of extinction and duration of the interaction prior to extinction for each parameter combination in the model with asexual reproduction strategy. Left panel: The number of simulations with extinction is indicated by the color intensity. The color indicates the number of extinctions for a total of 10 repetitions for each parameter combination. Right panel: Average time until the first extinction event. White squares indicate that coexistence occurred in all simulations. Parameters were: $K = 1500$, $L = 150$, $\mu = 0.0001$, $N_{gen} = 5000$.

3.2 ROBUSTNESS ANALYSIS

The qualitative patterns were robust to different parameter combinations. The patterns observed through replicates were invariable regardless of the parameter combinations. On the sexual reproduction model, increasing the carrying capacity did not change the coevolutionary dynamics, while increasing values of the mutation rate only resulted in a greater amplitude of both phenotype distributions. Oscillation patterns were found in all the evaluated genome sizes, however the oscillations were more conspicuous for smaller genomes than larger genomes (Supplementary Material 3, Figs. S3-S5). In

the asexual reproduction model, the evolutionary branching pattern and extinction were also observed for the different genome sizes (Supplementary Material 3, Figs. S6-S8).

The modeling of the phenotype as a continuous trait resulted in some differences when compared to the version that considered explicit genetic modeling. In the sexual reproduction model, the effect of decreasing the range of distribution of the exploiter phenotype with a higher interaction pressure on the exploiter was not observed (Supplementary Material, Fig. S9). In addition, the shift from a centralized to an oscillatory pattern was more strongly related to an increase in the interaction pressure on the exploiter than an increase in the strength of interaction on the victim. In the asexual model, both centralized patterns and evolutionary branching emerged from the interaction between exploiter and victim (Supplementary Material 4, Fig. S10). However, unlike the genetically explicit model, phenotypic variation in response to coevolutionary pressures occurred at a faster pace. While in the genetic model the cycle of branch formation would occur over hundreds of generations, in the model using continuous traits this cycle repeated itself in the scale of tens of generations. We also observed a coevolutionary pattern that was intermediate between the centralized pattern and the evolutionary branching (Supplementary Material 4, Fig. S11). In this scenario, the selective pressure exerted by the exploiter induced disruptive selection and favored extreme phenotype values on the victim, but it was not enough to completely separate its phenotypic distribution.

4 DISCUSSION

In this work we investigated coevolutionary patterns of antagonistic interactions and how the reproductive strategy and interaction pressure affected these outcomes on a genetically explicit model. Our simulations demonstrate that assumptions on sexual and asexual reproduction modes have important consequences on determining the evolutionary dynamics of the interaction. Specifically, given enough intensity on the interaction pressure, when sexual reproduction is assumed the antagonistic interaction results in oscillatory patterns of phenotype evolution. On the other side, asexual reproduction results in evolutionary branching associated with a high probability of extinction of the exploiter species. These results highlight the relevance of considering how genetic information and phenotypic traits are transmitted between generations in order to understand how ecological interactions can affect the evolutionary dynamics of antagonistic species.

Centralized and oscillatory patterns emerged as the results of the antagonistic interaction when individuals reproduce sexually. When the interaction pressure on either exploiter or victim was small, the selective pressure given by the interaction was not enough to cause changes in the evolutionary phenotypic trajectory of any species. Their phenotype distributions thus remained in stable and centralized values. However, a stronger interaction pressure on the exploiter imposed a cost on phenotype matching for the exploiter. Given that the exploiter phenotype followed a unimodal distribution, exploiters with phenotypes closer to the victim's most abundant phenotypes were favored. As a consequence, the phenotypic variance on the victim was reduced. These results support the predictions from other models in which coevolution restricts the phenotypic diversity of exploiters when they are selected to closely match their victim's phenotype (Frank, 1994; Yoder & Nuismer, 2010). At the same time, if the interaction pressure on the exploiter is increased, the coevolutionary patterns change from a centralized pattern to an oscillation in both species' phenotypes. The continuous cycles of increase and decrease on phenotypes have already been reported for numerous models of coevolutionary interactions in either single locus (Jayakar, 1970; Seger, 1988; Gavrillets & Hastings, 1998; Nuismer et al., 2003, Araujo et al., 2020) and multilocus quantitative models (Gavrillets, 1997; Nuismer et al., 2005; Kopp & Gavrillets, 2006). An important distinction from previous quantitative models, however, is regarding the regularity of the oscillations: While on those studies the oscillations were periodic with constant phenotype

oscillation amplitude, here the oscillations were irregular, as they are likely to respond to stochastic variations in the effects of selection given by the random choice of the victims and survival probabilities.

Changing the reproductive strategy from sexual to asexual resulted in a shift from oscillatory dynamics to evolutionary branching. As phenotypic homogenization was no longer present due to genetic recombination of the parent's genome, the selective pressure caused by the exploiter on intermediate phenotypes favored individuals on the victim population with phenotypes closer to the tails of the distribution. If the interaction pressure was strong enough, intermediate phenotypes on the victim were eventually excluded and its phenotype split into two branches. Evolutionary branching has already been reported for the parasite-host system (Calcagno et al., 2010) and other ecological interactions (Doebeli & Dieckman, 2000). In the former model, branches can remain stable depending on the mutation rates and interaction pressure on each species, and the exploiter and victim bifurcate in two pairs of phenotypically matching lineages. Cyclic episodes of phenotype bifurcation like the ones that emerged in our simulations have also been observed in this work. The second model presents evolutionary branching with either one or both species splitting their phenotypes distributions in two, that occurred when individuals reproduce asexually. Doebeli & Dieckman (2000) also demonstrated that this pattern can evolve when individuals reproduce via sexual reproduction where partner selection is related to positive assortative mating. In a mechanism that produces results similar to the ones observed for asexual reproduction, assortative mating favors individuals from the extremes of the phenotype distributions. As initially the interaction pressure penalizes those in the middle of the distribution, individuals on the tail of the distribution that mate with partners of close phenotype have higher fitness than those that reproduce with individuals with more distant phenotypes and produce offspring with intermediate values (Dieckmann & Doebeli, 2000). Both asexual reproduction and sexual reproduction via assortative mating break the homogenization of phenotypes, which creates the opportunity for divergent selection and the emergence of character bifurcation. It is possible that the inclusion of assortative mating in our model can lead to similar patterns, although this hypothesis should be better investigated in future studies.

A distinct behavior from our model is that while the coexistence of both species was persistent if interaction pressure was weak, in most cases the disruptive selection that emerged on the asexual model resulted in the extinction of the exploiter. The emergence of two distinct phenotypic clusters led the exploiter population to specialize in

just one of the branches (Doebeli, 1996b). After one of them was extinguished, the exploiter was no longer able to successfully use the other phenotypes. Thus, the emergence of branching became deleterious for the exploiter, while allowing the victim to escape the interaction. Interestingly, this result parallels a pattern that has been documented in *Daphnia* attacked by the yeast parasite *Metschnikowia bicuspidata*, where both species display asexual reproduction modes (Duffy et al., 2008). The invasion of the yeast on this system led to the formation of a bimodal phenotypic distribution of the victim's traits, followed by a disappearance of the parasite species. While the study does not explore the reason that led to the local extinction of the parasite population, a possible explanation could be the failure of the parasite in coping with the phenotype divergence induced by the interaction.

For both reproductive modes, the frequency-dependent selection was an important process regulating the phenotype frequency of each species (Lande, 1976; Sinervo & Calsbeek, 2006). Similar to systems in which a parasite's frequency is strongly selected to match the most abundant host genotype (Siemens & Roy, 2005; Koskella & Lively, 2009), in our model the exploiter's phenotype was favored when attacking the most common phenotypes in the victim population. In turn, this adaptation of the exploiter results in an advantage for the less common victim phenotypes and increases their frequency (Haldane, 1949; Hamilton, 1980). Such dynamics result in a time-lagged variation of the exploiter phenotype that was continuously selected to track the most abundant victim phenotypes (Hutson & Law, 1981; Kopp & Gravilets, 2006), an essential feature that characterizes parasite-host arms-race (Dybdahl & Lively, 1998).

The evolutionary outcomes depended on how the offspring receives genetic information. On the sexual reproduction strategy, the offspring inherits half of each parent's genotype (Taper & Case, 1985). As a consequence, its phenotype has a greater probability of assuming an intermediate value between both parents' phenotypes, and the "reshuffling" of their genomes determines the phenotypic distribution on the next generation when mating is random (Doebeli, 1996a; Doebeli & Dieckman, 2000). Also, the phenotype frequency usually assumes a normal-like distribution. For the asexual reproduction strategy, the phenotype is equal to the parent's phenotype plus a variation caused by a mutation on each locus. As a consequence, phenotypes equal or close to the ones that remained on the previous generation have their frequency amplified on the next generation. The variation of phenotype between the offspring and its parent's phenotype is smaller when compared to the models where sexual reproduction takes

place. At the same time, the phenotype of the populations is not restricted to normal-like distribution, and multimodal shapes can emerge depending on the fitness differences that occur along the phenotypic space. These differences in the outcomes of each reproductive strategy have important evolutionary implications, as detailed below.

First, sexual reproduction allowed the interaction to persist, while asexual reproduction had deleterious results for the exploiter species. In our model, we investigated the effects of reproductive strategy (and recombination) for quantitative traits that are controlled by additive effects of multiple loci (Lynch & Walsh, 1998). The reproductive strategy was a key determinant of phenotype distribution of one generation to the next, as a function of the genomes and phenotypes of surviving individuals of the previous generation. For the victim, even high levels of interaction pressure did not result in the population extinction, so its persistence was maintained for both types of reproductive strategy. However, the reproductive strategy of the victim resulted in two very distinct coevolutionary patterns, characterized by either presence or absence of branching in its phenotype distribution. For the exploiter, the absence of bifurcation allowed it to track the victim's phenotype and persist even in strict conditions of high interaction pressure. But if the phenotype distribution bifurcated into two distinct groups, specialization on one of the branches resulted in most cases in its extinction due to its inability to successfully attack the remaining victims after depleting the individuals on one branch. Here, the persistence of the exploiter was highly related to the coevolutionary dynamics that emerged within each strategy, including the mechanism of reproduction on the exploited species.

Second, the aspects we observed in our model also have relevant implications for studies of sympatric diversification and speciation induced by ecological interactions. Models of sympatric speciation assume that speciation can arise when a population experiences divergent character selection if that character is directly or indirectly linked to mating behavior and reproductive isolation (Dieckmann & Doebeli, 1999). Therefore, evolutionary branching is an important component of models that investigate sympatric speciation events, and a necessary step that precedes reproductive isolation (Dieckmann & Doebeli, 1999; Doebeli & Dieckman, 2000). In our model, we show that stable evolutionary branchings are unlikely outcomes of the interactions in either sexual or asexual reproductive strategies. As a consequence, pairs of antagonistic interactions are not expected to result in speciation in genetically explicit models if the interaction is the only source of divergence of the populations. The sexual reproduction prevented the

emergence of branching by converging the population's phenotype to a unimodal distribution. On the asexual model, evolutionary branching was an unstable pattern that resulted in cycles of bifurcation in the victim's phenotype or extinction of the exploiter's population. Doebeli & Dieckman (2000) found stable patterns of evolutionary branching, and Araujo et al., (2020) found scenarios with different periods of persistence of branches. Given such distinct outcomes regarding the persistence of evolutionary branches, we conclude that long-term persistence of evolutionary branching can be less common than previously assumed.

Finally, explicitly modeling the genetic basis of quantitative traits showed some key differences when compared to the alternative model without the explicit modeling of the genome. Although we found the same qualitative patterns of coevolutionary dynamics when traits were considered as continuous traits, specific aspects of the dynamics were not mutually present on both versions. For example, on the alternative model, the phenotypic variability on the exploiter was not reduced in comparison to the variability found on the victim, even for strong interaction pressure. Also, the asexual reproductive strategy was also more stable for weak interaction pressure, as we observed incipient branching on the victim phenotypes that allowed the persistence of the exploiter population. This pattern was not observed in the genetically explicit model even for small interaction pressure on the victim. We believe that these differences can be better understood by examining the assumptions that are required for each model and its consequences. First, on the alternative model, the effect of variation due to mutation acts directly on the phenotype value, and the Gaussian distribution that gives the probability of phenotype variation is symmetric for any direction. When the genome is modeled explicitly, variations on the phenotype depend on the sum of the variations given by a mutation probability in each locus. Thus, the final variation in phenotype values depends on the genome size and the ratio between the frequency of each binary value in the genome, as there is a greater probability that the sum of all values approaches half of the genome size. Second, on the alternative model, the offspring phenotype on the sexual reproductive strategy is simplified in order that it is equal to the mean of both parents' phenotype plus the probability of mutation. On the genetically explicit model, recombination produces greater variation in the offspring fitness that is linked to the number of non-overlapping loci values on each parent (Doebeli, 1996). Finally, modeling traits as continuous values presents the problem that coevolution can potentially drive traits to unrealistic infinite values (Kopp & Gavrillets, 2006). This was circumvented by

including an additional parameter of external stabilizing selection (Gavrilets & Hastings, 1998), an assumption that is not necessary when modeling multilocus models of quantitative traits as the maximum phenotype value is restricted by the length of the genome.

Although we believe that our approach allows us to make general predictions on the expected outcomes according to different reproductive strategies, we outline some important potential limitations of the model. The selection of the victim was random and independent of its trait value, although in nature empirical evidence shows that parasites, phytophagous insects and predators can display preference behavior according to its victim trait (Nylin et al., 2005; Soler et al., 2014; Jorge et al., 2014; Nagarajan et al., 2015). Selection on the victim can produce unexpected coevolutionary patterns on specific conditions (Araujo et al., 2020). Another assumption of the model is that generations of both exploiter and victim were considered as discrete and their generation time was equal. Relative differences in generation time from parasites and hosts can accelerate their adaptation to the host (Gandon & Michalakis, 2002, but see Morgan & Buckling, 2006) and affect coevolutionary dynamics (Calcagno et al., 2010). Sexual mating also did not include assortative mating, which has potentially important consequences of the results of the coevolutionary dynamics (Doebeli & Dieckman, 2000). Finally, demographic variation due to the interaction (Papkou et al., 2016) or variations in growth rates according to the reproductive strategy (Smith, 1978; Michod & Levin, 1988; Otto & Lenormand, 2002) were not considered. To address the effects of these assumptions on the outcomes of the model represents promising avenues of exploration of future studies.

In summary, our model investigates the expected coevolutionary dynamics when finite populations of antagonistic species interact assuming that the interaction is mediated by quantitative traits with explicit genomes. The coevolutionary dynamics were largely affected by the reproduction mode of the species, leading either to the coexistence or extinction of the exploiter species. Given the ubiquity of sexual reproduction strategy on nature, our work suggests that explicitly evaluating the effects of sex can have relevant impacts on the prediction of coevolutionary dynamics and the maintenance of sexual reproduction in natural populations.

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SUPPLEMENTARY MATERIAL 1

Here a few of the design concepts that were used to build the model, following recommendations of the ODD protocol (Grimm et al., 2006; Grimm et al., 2010).

Emergence: The genome of the offspring and phenotype values emerge from the explicit description of the genome. The phenotype of the population along with generations changes due to mutation, demographic drift, and individual fitness mediated by the interaction pressures.

Adaptation: it is not explicitly modeled, as the identity of the victim that an exploiter interacts with is chosen randomly. Therefore, there is no explicit behavior that maximizes the chance of survival of any individual. On the other hand, the phenotypic distribution of each population emerges as an outcome of the interactions and survival of the previous generation. The offspring inherits phenotypic values that are close to its parents and are likely to present phenotype values in ranges that received less selective pressure in the last interactions.

Objectives: Fitness is modeled explicitly as the probability of survival after the interactions. Individuals and their phenotype values are selected according to the interaction pressure, which depends on the phenotypic difference of the interacting individuals. The fitness of the exploiter is higher when its phenotype values are close to the phenotype of the exploiter. The fitness of the victim decreases according to the number and strength of the interactions that it has received from the exploiter. The success of each individual results in its survival and the opportunity to reproduce and generate offspring to the next generation.

Interaction: exploiters interact with their victims by selecting one of them as a “host”. This interaction results in the exploiter’s fitness and a decrease in the victim’s fitness. If the reproduction is sexual, individuals from the same trophic level also interact with mating partners so that the offspring carries 50% of each parent’s genome.

Stochasticity: the identity of the victim chosen by the exploiter is assigned randomly. Also, the identity of the parent and the mating pair is also chosen by chance with equal probability. In the sexual selection model, the probability is inversely proportional to the phenotypic distance. Each locus inherited by the offspring has a 50% chance to be inherited by one of the parents, and the mutation occurs with a probability set by a mutation rate. Survival is also a product of chance since each individual survives with a survival probability that is given by its fitness value.

Collectives: individuals from each trophic level are considered as one population. The phenotype distribution in each generation that is used to describe the results of the evolutionary dynamic from the frequency of phenotypes in each population.

Observation: for each 5-time step, it is recorded the phenotype frequency of all individuals from both exploiter and victim populations. This data is plotted to depict the patterns of phenotype distribution along time.

SUPPLEMENTARY MATERIAL 2

Coevolutionary dynamics for a range of parameter combinations regarding interaction pressure for the exploiter (alpha) and victim (beta) species. Parameters were: $K = 1500$, $L = 150$, $\mu = 0.0001$, $N_{gen} = 1500$.

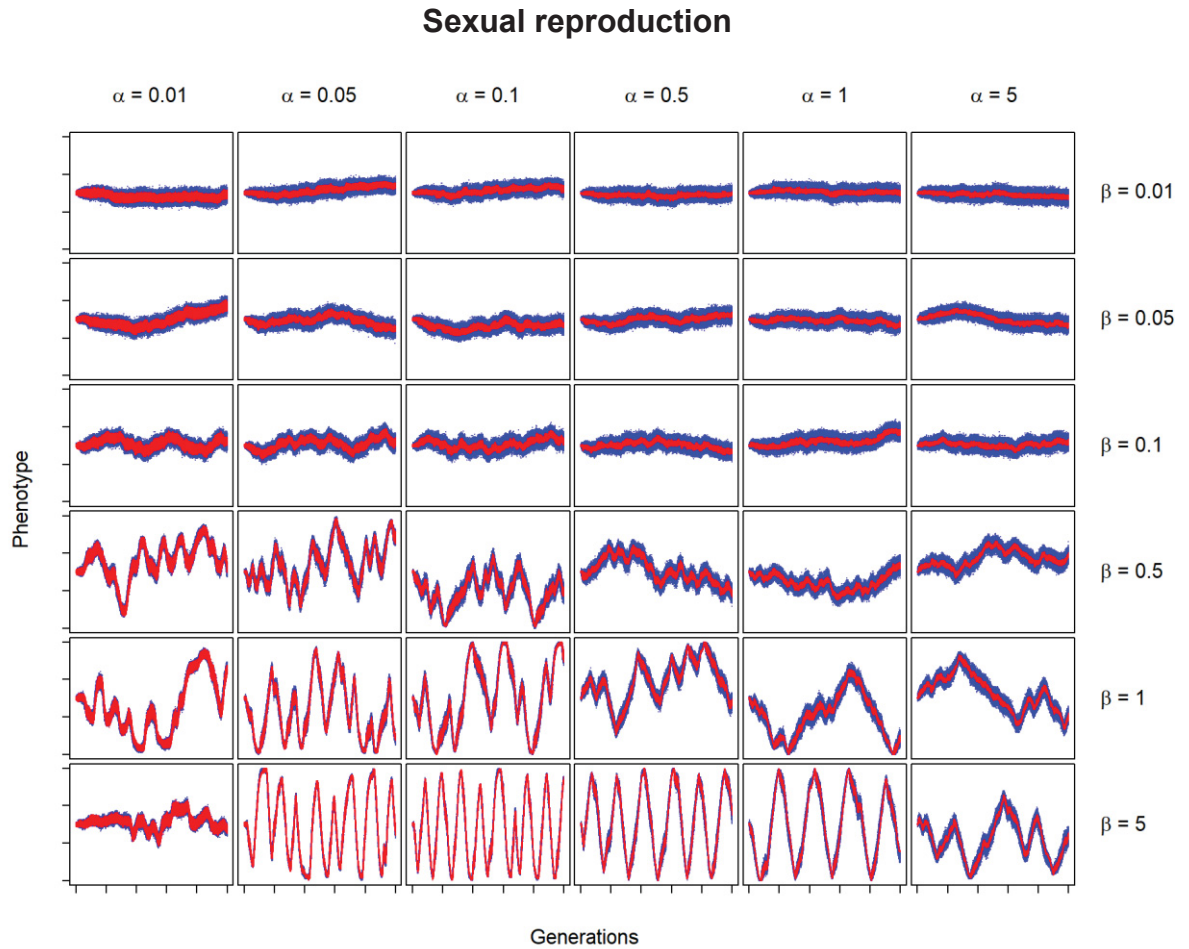


Figure S1. Coevolutionary dynamics for the exploiter (red) and victim (blue) along with generations for the model with sexual reproduction. Increasing values of interaction pressure for the exploiter (alpha) and victim (beta) leads to more oscillation in the phenotypic dynamics resulting from the interaction. For each panel, generations (x-axis) ranges from 0 to 1500, and phenotype values (y-axis) from 0 to 150.

Asexual reproduction

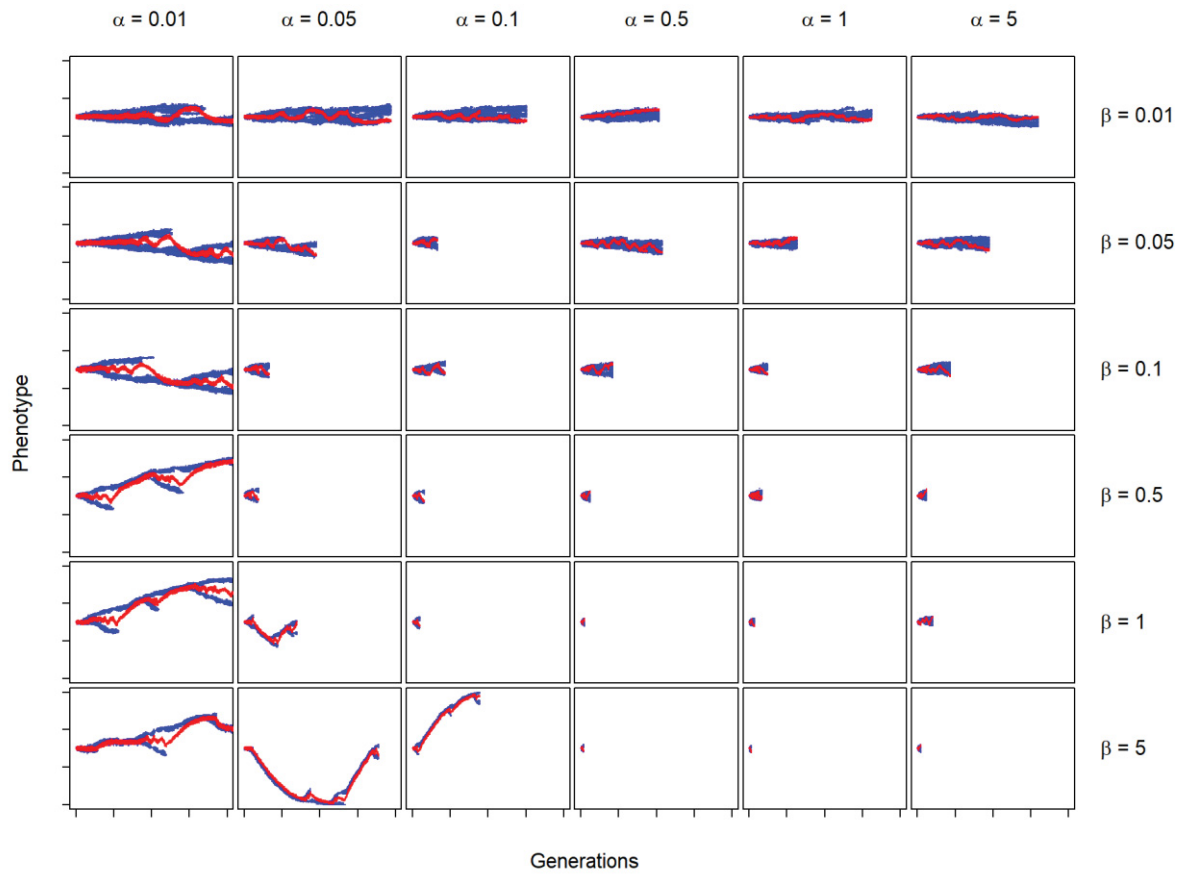


Figure S2. Coevolutionary dynamics for the exploiter (red) and victim (blue) along with generations for the model with asexual reproduction. Increasing values of interaction pressure for the victim (beta), while the interaction pressure on the exploiter (alpha) is low (first column) results in evolutionary branching. Increasing the interaction pressure on the exploiter results in extinction of the interaction. For each panel, generations (x-axis) ranges from 0 to 1500, and phenotype values (y-axis) from 0 to 150.

SUPPLEMENTARY MATERIAL 3

Here it is shown the coevolutionary dynamics for different genome sizes (L). The results indicate that the coevolutionary dynamics follow a similar trend for most of the different genome sizes that were evaluated. An exception occurs in the sexual reproduction model for the largest genome size ($L = 500$), where the centralized pattern occurs more frequently than the oscillatory pattern. In this scenario, it is possible that the effect of phenotypic variation due to mutation in the genome exceeds the effect of variation caused by selection due to the interaction.

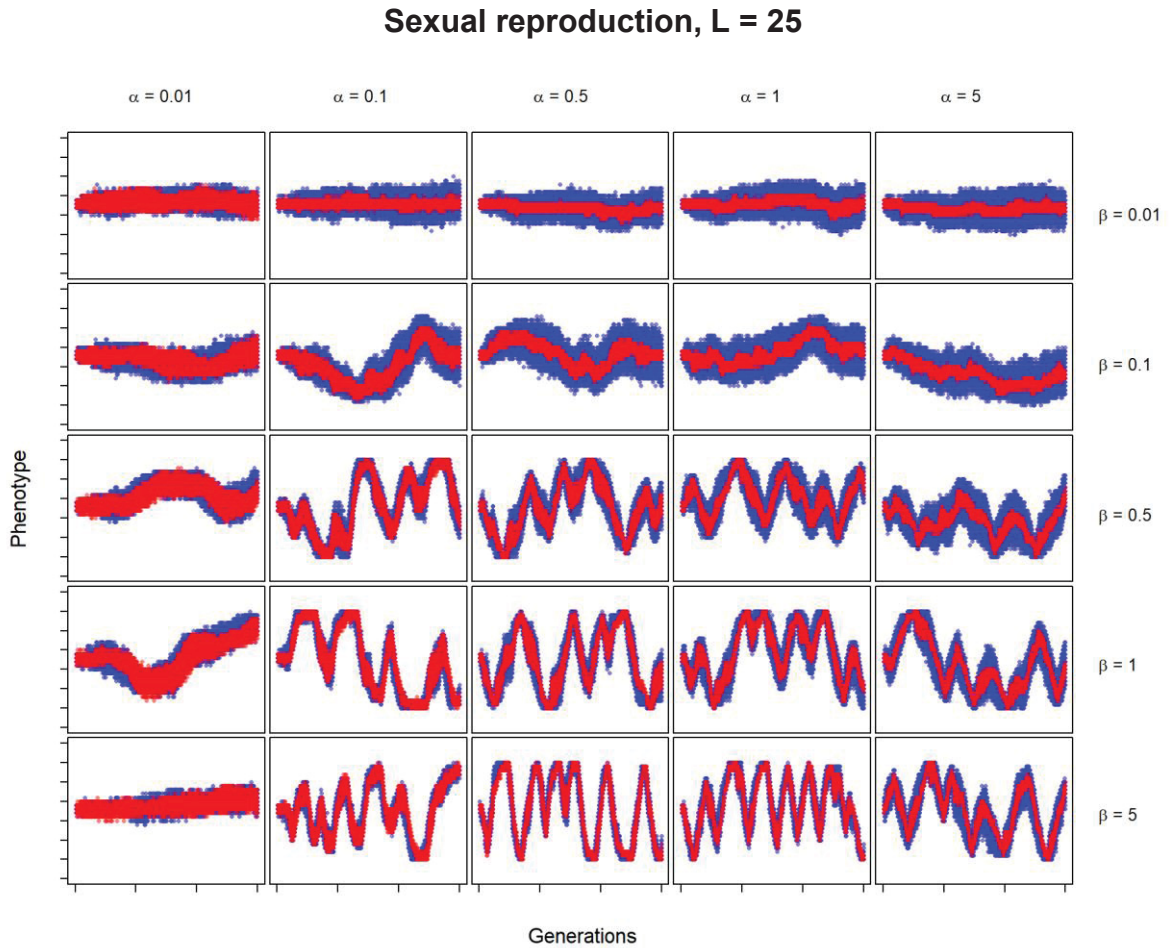


Figure S3. Coevolutionary dynamics for the exploiter (red) and victim (blue) along with generations for the model with sexual reproduction. Increasing values of interaction pressure for the exploiter (alpha) and victim (beta) leads to more oscillation in the phenotypic dynamics resulting from the interaction. For each panel, generations (x-axis) ranges from 0 to 1500, and phenotype values (y-axis) from 0 to 25. Parameters were: $K = 1500$, $\mu = 0.0001$, $N_{gen} = 1500$.

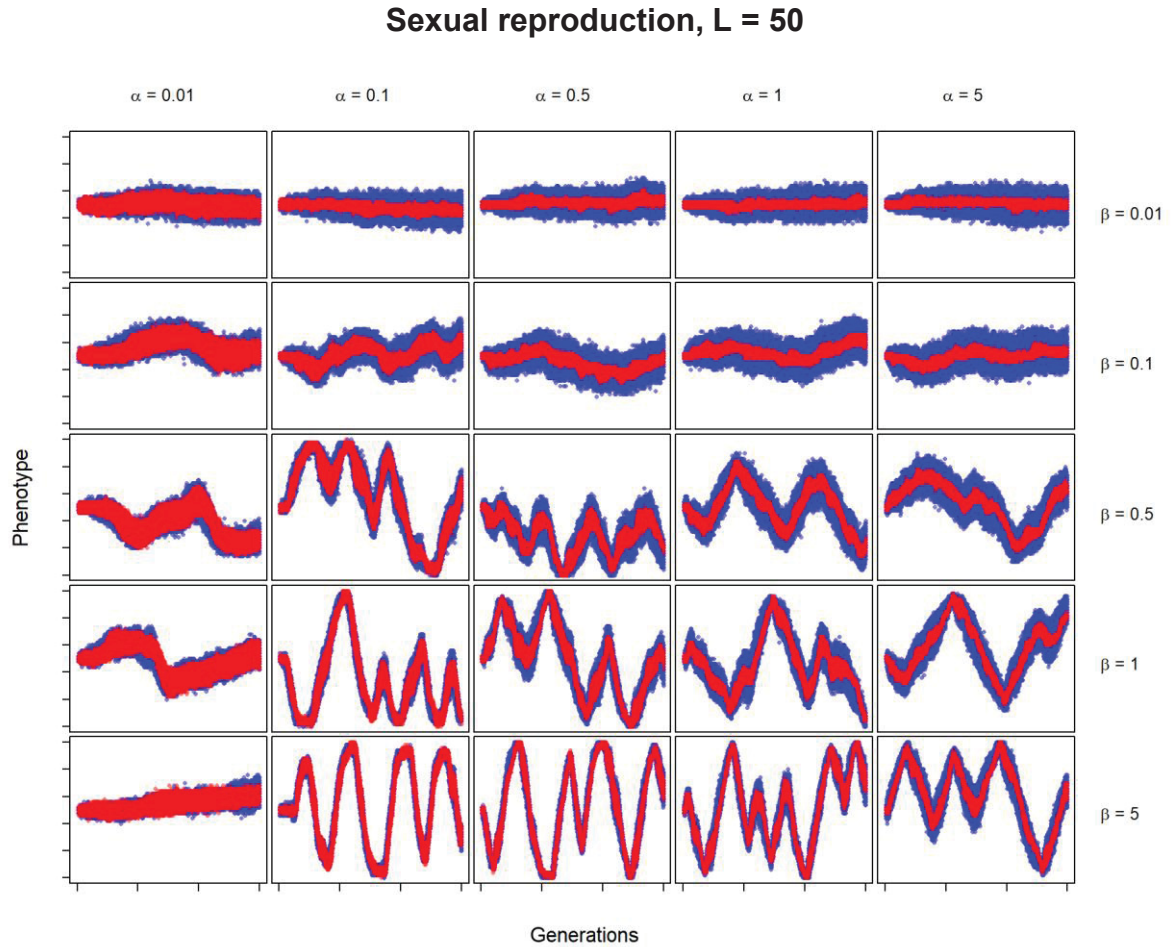


Figure S4. Coevolutionary dynamics for the exploiter (red) and victim (blue) along with generations for the model with sexual reproduction. Increasing values of interaction pressure for the exploiter (alpha) and victim (beta) leads to more oscillation in the phenotypic dynamics resulting from the interaction. For each panel, generations (x-axis) ranges from 0 to 1500, and phenotype values (y-axis) from 0 to 50. Parameters were: $K = 1500$, $\mu = 0.0001$, $N_{gen} = 1500$.

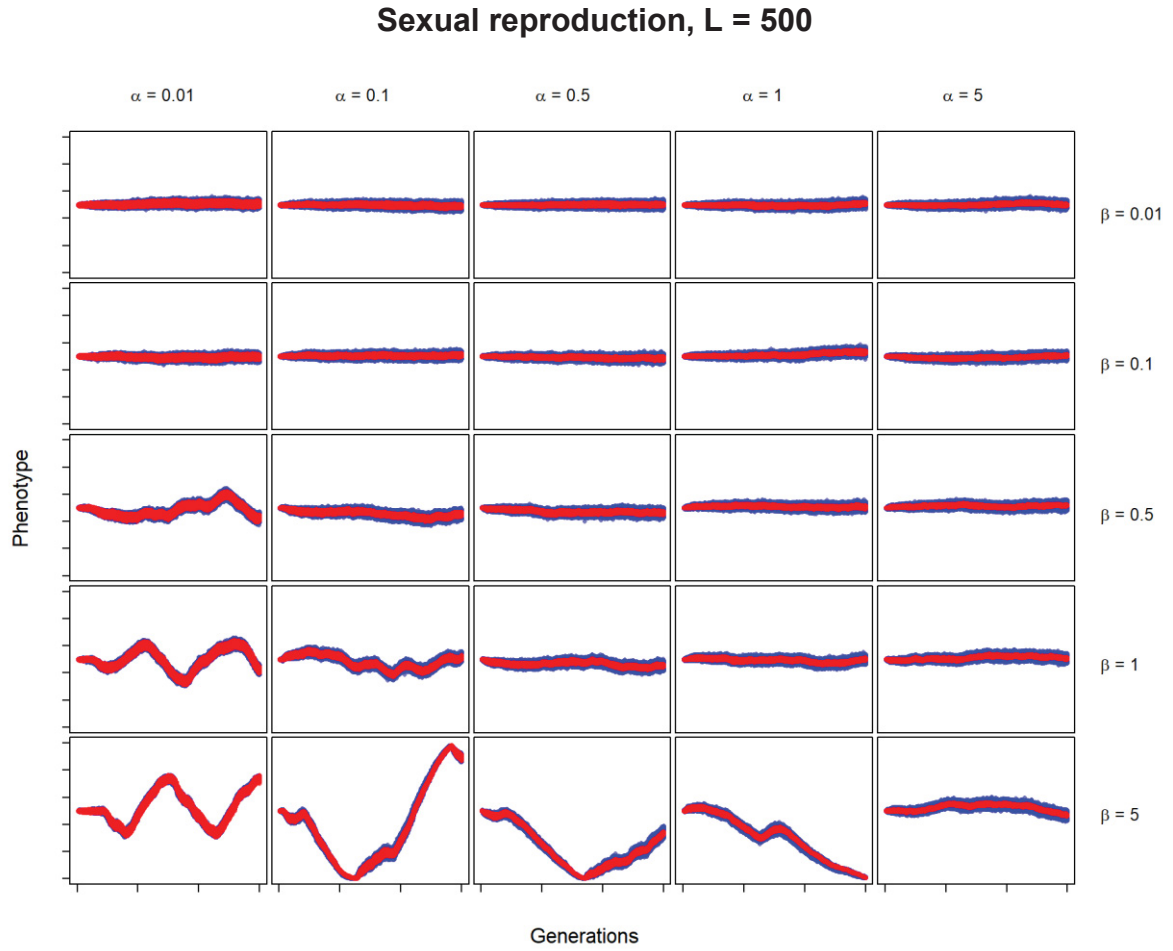


Figure S5. Coevolutionary dynamics for the exploiter (red) and victim (blue) along with generations for the model with sexual reproduction. Increasing values of interaction pressure for the exploiter (alpha) and victim (beta) leads to more oscillation in the phenotypic dynamics resulting from the interaction. For each panel, generations (x-axis) ranges from 0 to 1500, and phenotype values (y-axis) from 0 to 500. Parameters were: $K = 1500$, $\mu = 0.0001$, $N_{gen} = 1500$.

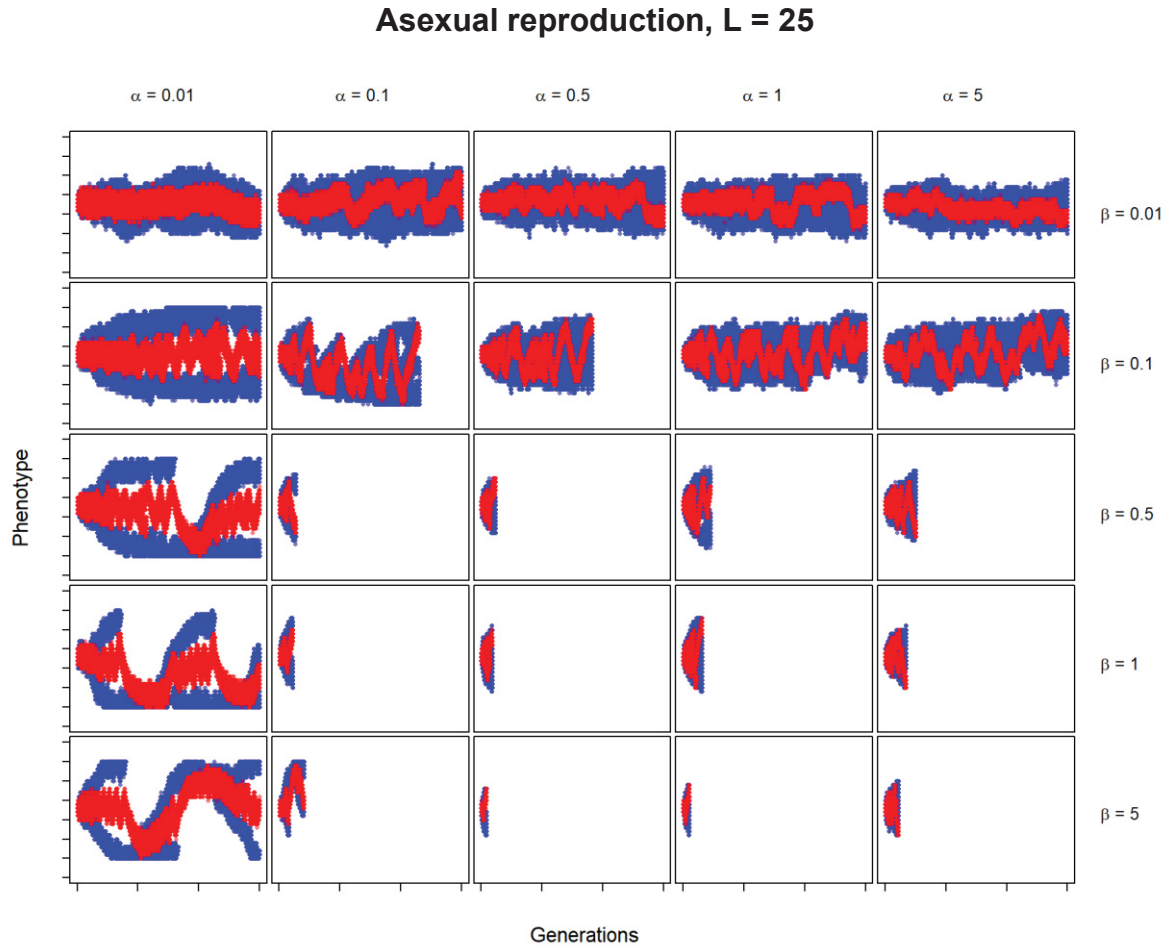


Figure S6. Coevolutionary dynamics for the exploiter (red) and victim (blue) along with generations for the model with asexual reproduction. For lower values of interaction pressure for the exploiter (alpha) or victim (beta), the phenotype of the victim results in evolutionary branching. Increasing the strength of interaction pressure in either species results in extinction of the interaction. For each panel, generations (x-axis) ranges from 0 to 1500, and phenotype values (y-axis) from 0 to 25. Parameters were: $K = 1500$, $\mu = 0.0001$, $N_{gen} = 1500$.

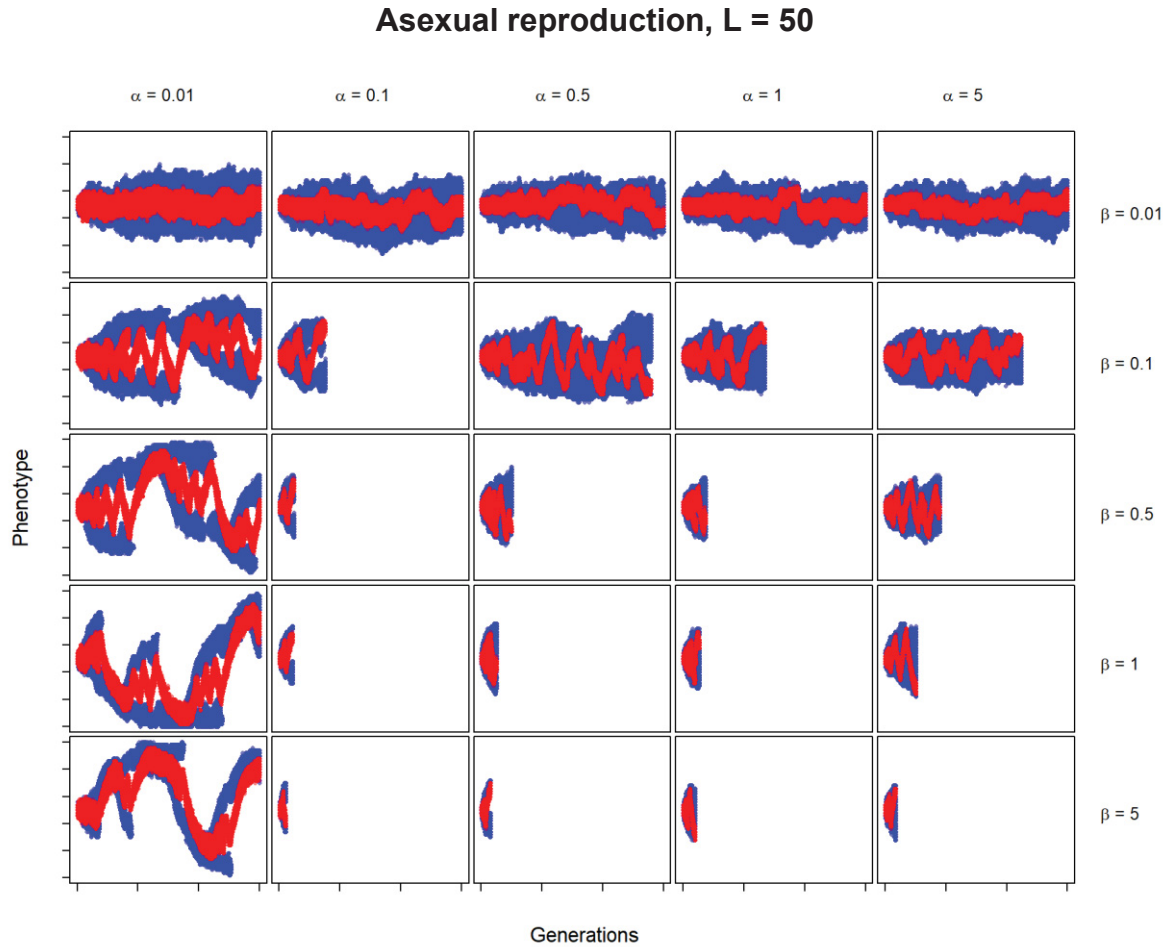


Figure S7. Coevolutionary dynamics for the exploiter (red) and victim (blue) along with generations for the model with asexual reproduction. For lower values of interaction pressure for the exploiter (alpha) or victim (beta), the phenotype of the victim results in evolutionary branching. Increasing the strength of interaction pressure in either species results in extinction of the interaction. For each panel, generations (x-axis) ranges from 0 to 1500, and phenotype values (y-axis) from 0 to 50. Parameters were: $K = 1500$, $\mu = 0.0001$, $N_{gen} = 1500$.

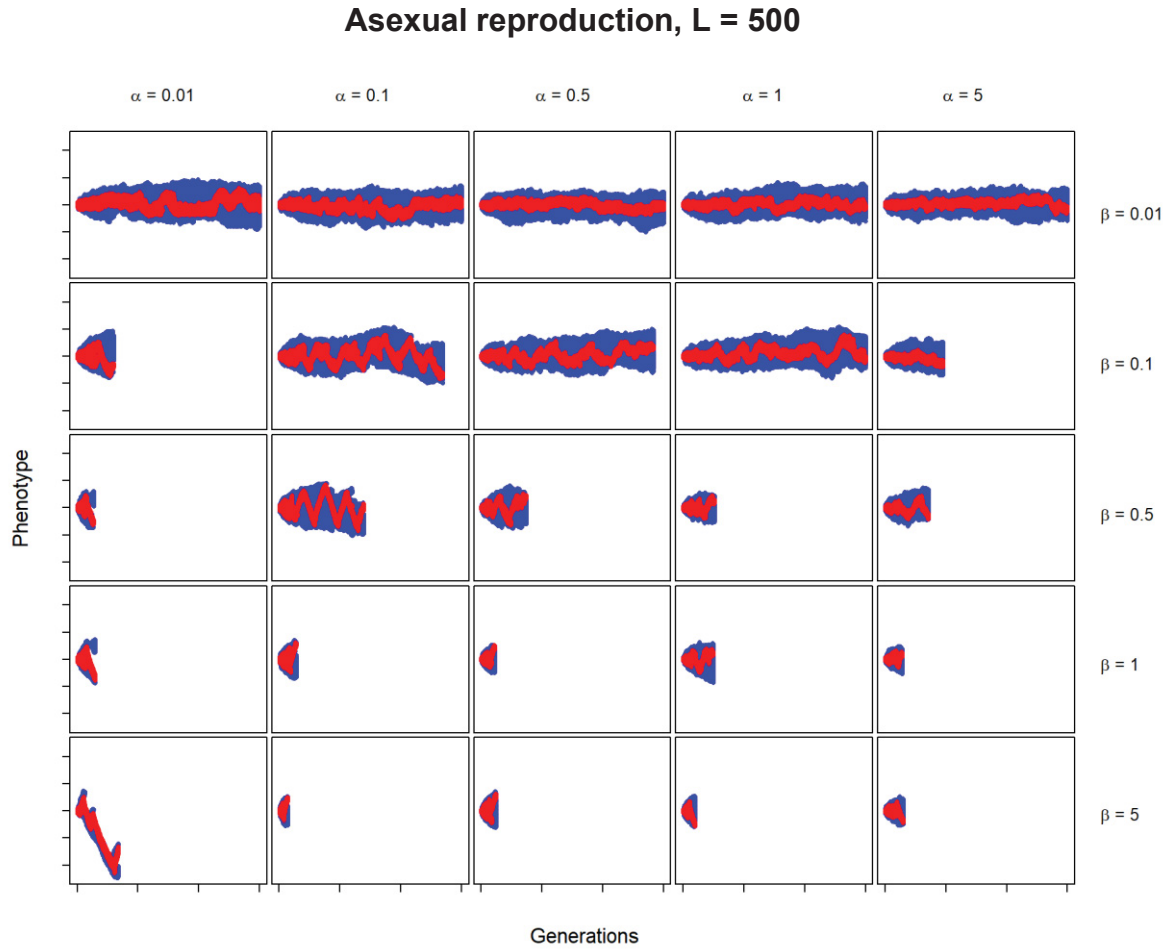


Figure S8. Coevolutionary dynamics for the exploiter (red) and victim (blue) along with generations for the model with asexual reproduction. For lower values of interaction pressure for the exploiter (alpha) or victim (beta), the phenotype of the victim results in evolutionary branching. Increasing the strength of interaction pressure in either species results in extinction of the interaction. For each panel, generations (x-axis) ranges from 0 to 1500, and phenotype values (y-axis) from 125 to 375. Parameters were: $K = 1500$, $\mu = 0.0001$, $N_{gen} = 1500$.

SUPPLEMENTARY MATERIAL 4

Here it is shown the coevolutionary dynamics when the genome is not explicitly modeled. Phenotypes are represented by real positive or negative numbers. Since the scale of phenotypic variation is different from the model that includes explicit genetic modeling of the individuals, the parameters used in these simulations are detailed below.

Table S1. List of parameters used in the model with a short description of their meaning.

Parameter	Description	Value
K	Carrying capacity	1500
δ	Standard deviation for phenotypic variation due to reproduction	0.2
θ_{otm}	Phenotype value favored by the stabilizing pressure	0
α	Interaction pressure on exploiters	1, 4, 16,64, 256
β	Interaction pressure on victims	1, 4, 16,64, 256
γ	External stabilizing pressure	0.1

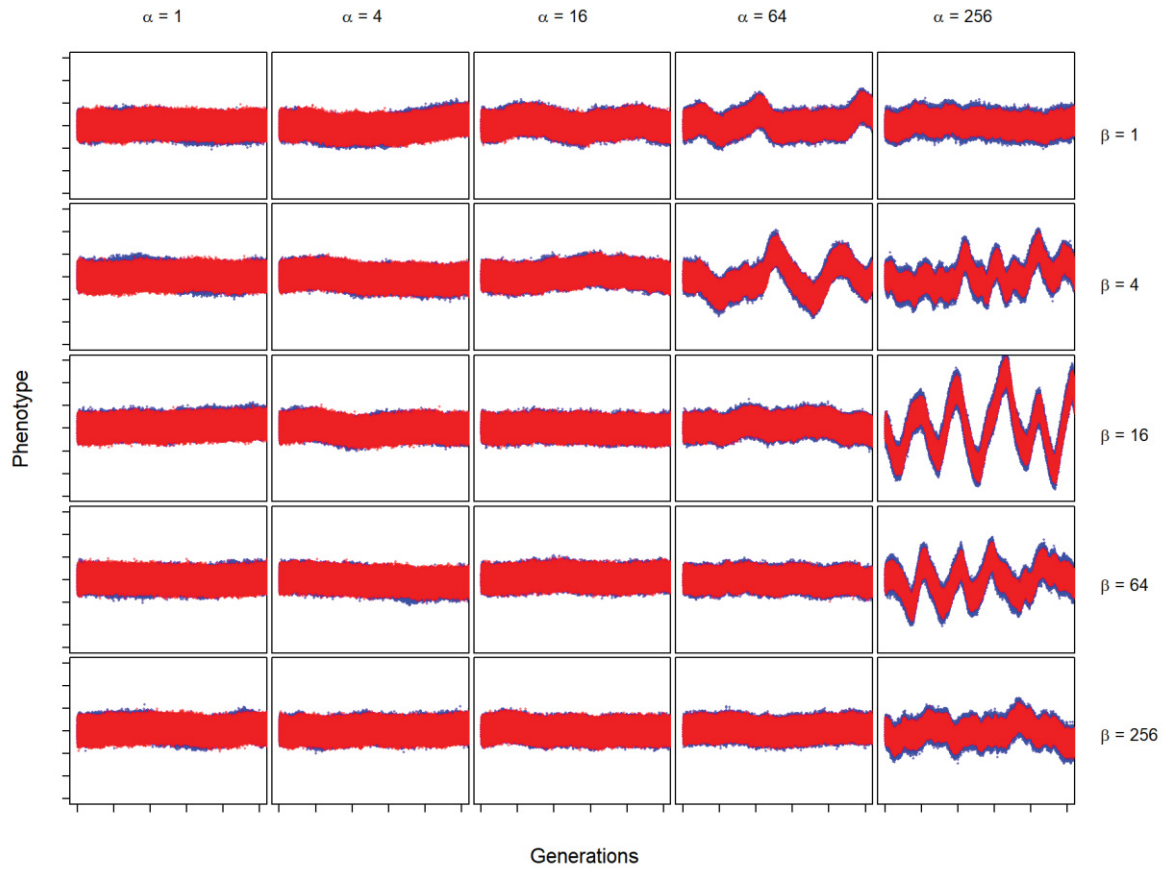


Figure S9. Coevolutionary dynamics for the exploiter (red) and victim (blue) along with generations for the model with sexual reproduction without explicitly modeling the genome. Lower values of interaction pressure on the exploiter (alpha) resulted in a centralized pattern of phenotypic distributions. Oscillations in the phenotypic dynamics were observed only for higher intensities in the interaction pressure for the exploiter (alpha). For each panel, generations (x-axis) ranges from 0 to 1000, and phenotype values (y-axis) from -1.0 to 1.0. Parameters were: $K = 1500$, $\gamma = 0.1$, $\theta = 0.02$, $N_{gen} = 1000$.

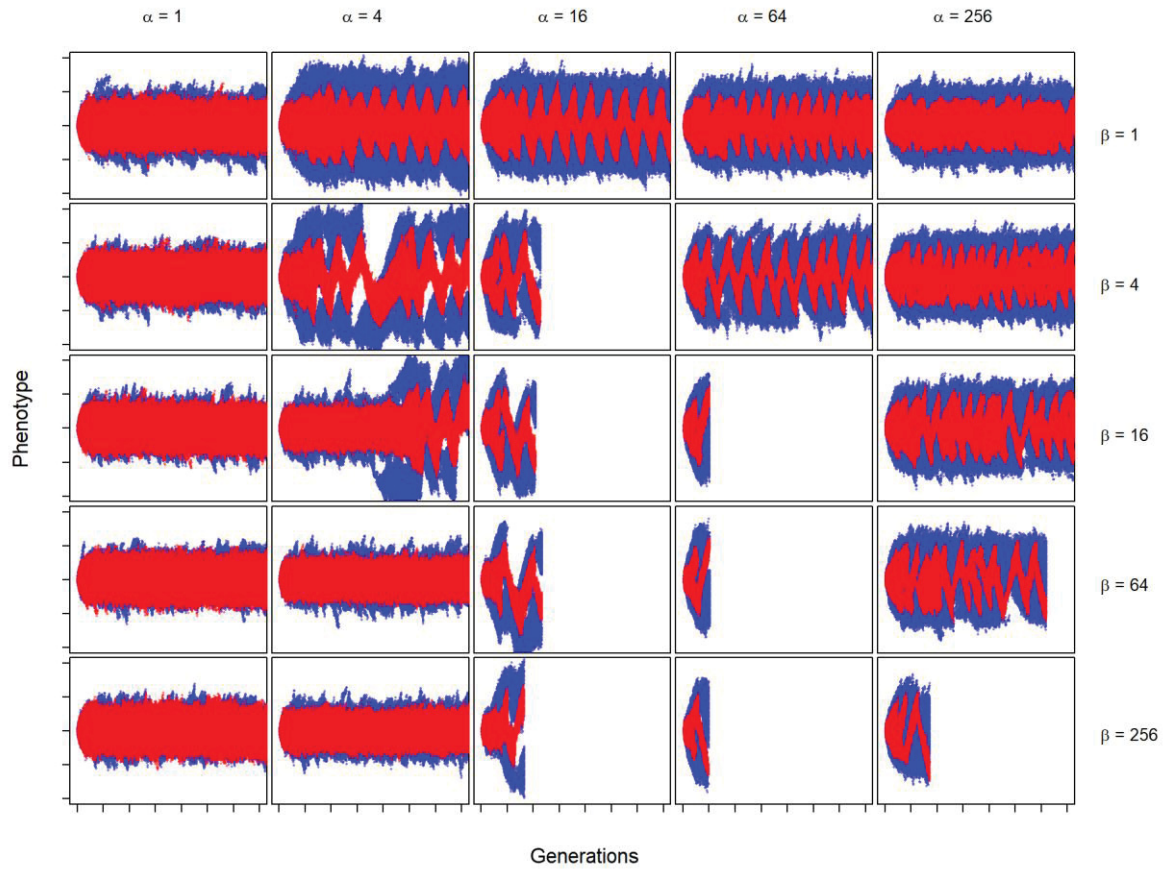


Figure S10. Coevolutionary dynamics for the exploiter (red) and victim (blue) along with generations for the model with asexual reproduction without explicitly modeling of the genome. It is possible to observe the centralized pattern, incipient branching, evolutionary branching and evolutionary branching followed by extinction. For each panel, generations (x-axis) ranges from 0 to 350, and phenotype values (y-axis) from -0.6 to 0.6. Parameters were: $K = 1500$, $\gamma = 0.1$, $\theta = 0.02$, $N_{gen} = 350$.

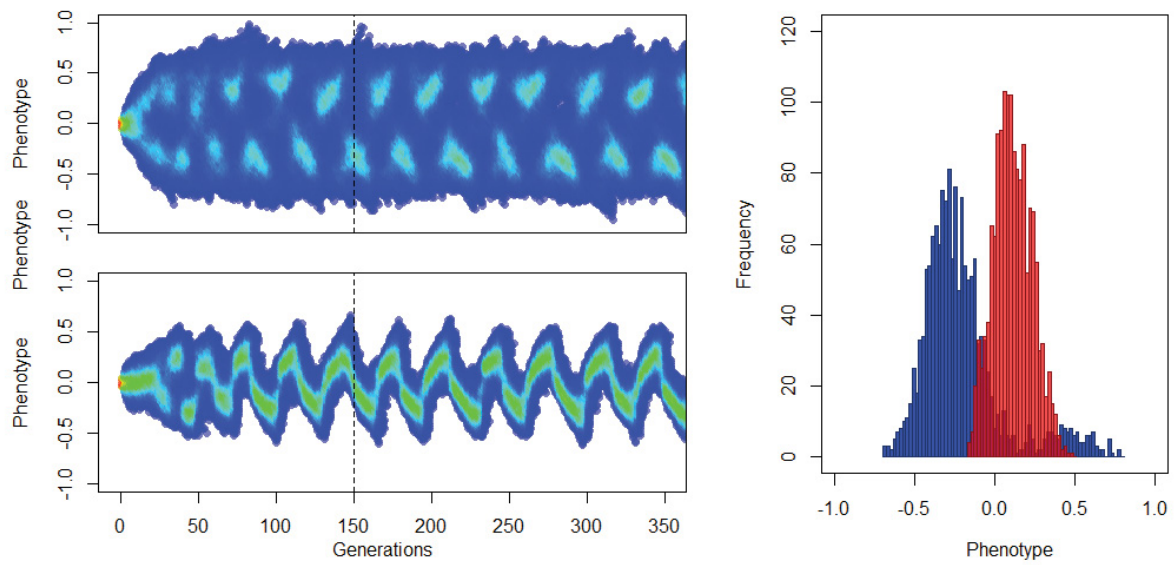


Figure S11. Incipient evolutionary branching pattern, when individuals reproduce asexually without explicitly modeling the genome. The left panel depicts the phenotype evolution throughout generations for victim (above) and exploiter (below). The right panel shows the frequency of individuals with each phenotype for both exploiter and victim populations at one particular generation (dotted line at the left panels). exploiters are represented in blue, while victims are represented in red. Parameters were: $K = 1500$, $\alpha = 16$, $\beta = 1$, $\gamma = 0.1$, $\theta = 0.02$, $N_{gen} = 350$.

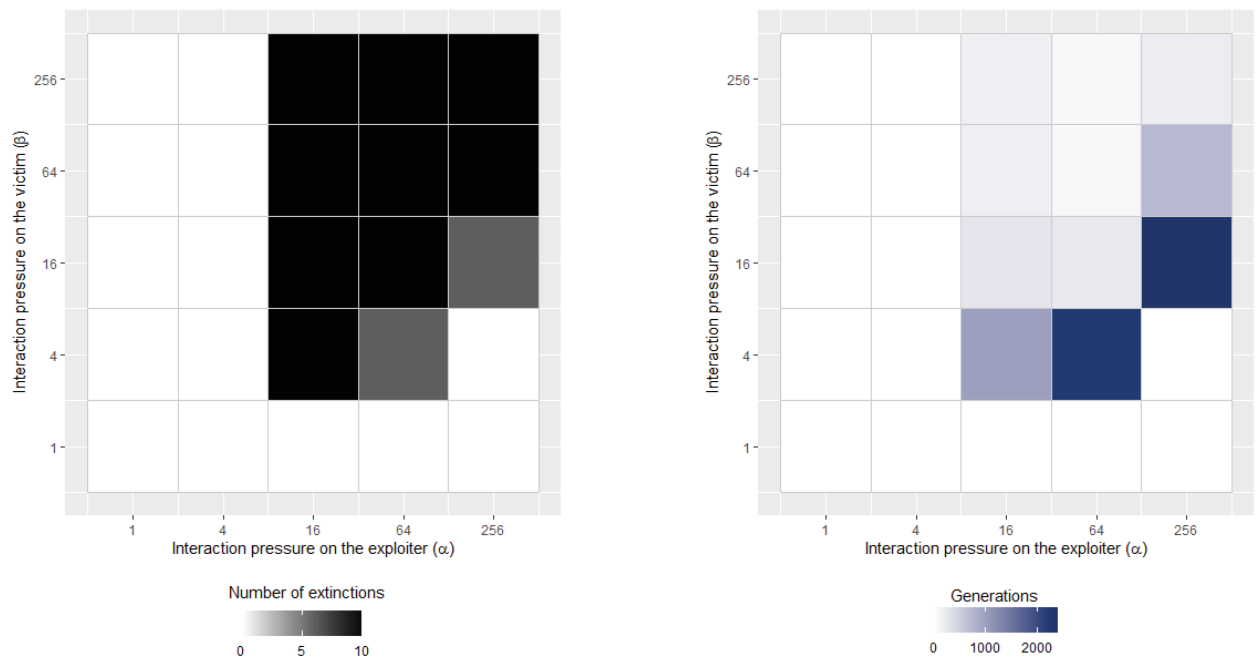


Figure S12. Frequency of extinction and duration of the interaction prior to extinction for each parameter combination in the model with asexual reproduction strategy without explicitly modeling of the genome. A. The frequency of simulations with extinction is indicated by the color intensity. The color indicates the number of extinctions for a total of 10 repetitions for each parameter combination. B. Average time until the first extinction event. White squares indicate that coexistence occurred in all simulations. Parameters were: $K = 1500$, $\gamma = 0.1$, $\theta = 0.02$, $N_{gen} = 5000$.

CAPITULO 3

THE ROLE OF SPACE AND SELECTION IN HOST RANGE OSCILLATIONS AND DIVERSIFICATIONS

The role of space and selection in host range oscillations and diversifications

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ABSTRACT

The prominent diversity observed in plant-feeding insects and parasites has led to the development of several evolutionary hypotheses regarding the processes that drive the species richness in these groups. Despite the broad theoretical and empirical support of the role of the host in the diversification of herbivorous insects, processes such as geographic isolation can contribute concomitantly to the formation of this richness. To investigate how geographic isolation interacts with host use in processes of species diversification and evolution, we propose an Individual-Based Model of organisms with explicit genomes in a spatial context. Individuals reproduce sexually with partners restricted by thresholds for genetic differentiation and geographical proximity. The individuals' fitness is given the compatibility of their phenotype with a favored phenotype imposed by the host. Species are defined as groups isolated by limited gene flow, and their host range is given by the realized interactions in each generation. We analyzed the result of the simulations by varying the intensity of the selective pressure and the size of the dispersion radius of the individuals. Higher selective pressure and smaller dispersion radius interacted to produce greater species richness while decreasing the average host repertoire size. Lineages experience phases of expansion of their host range, and speciation events resulted in different changes in the level of specialization for each new pair of lineages. The dynamics that emerge from the model are compatible with the theoretical framework given by the Oscillation Hypothesis and contribute to a better understanding of the role of interaction between biotic interactions and spatial distribution in diversification processes.

Keywords: Individual-based modeling. Diversification. Interactions. Speciation. Oscillation Hypothesis.

1 INTRODUCTION

Plant-feeding insects and parasites comprise much of the diversity of life (Mitter et al., 1988; Price, 1980). Understanding the different factors that drive the diversity of these groups is consequently an important step in elucidating global patterns of biodiversity. Both groups are characterized by intimate associations, in which they live at the expense of their hosts in at least one stage of their life cycle (De Meeûs & Renaud, 2002). Most of these associations are presently restricted to just one or a few hosts (Forister et al., 2015), and the great number of specialists in these groups suggests that ecological specialization can be an important factor related to the observed diversification of these organisms. Indeed, evidence suggests that processes related to variation in host range play a fundamental role in promoting their diversity, although it is debated how different mechanisms can act and influence this process (Erich & Raven, 1964; Thompson, 2005; Janz & Nylin, 2008; Fordyce, 2010; Hardy & Otto, 2014; Edger et al., 2015).

For many decades, traditional diversification hypothesis suggested that patterns of host specialization were the result of a process of continuous selection on specialization along evolutionary time (Moran, 1988; Wiegmann et al., 1993; Kelley & Farrell, 1998). This view relies on the assumption that the performance on different hosts is ruled by adaptive trade-offs, where specialized organisms increase their performance on one resource while decreasing their ability to successfully use others (Joshi & Thompson, 1995; Futuyma & Moreno, 1988). The intimacy and persistence of these interactions would result in high levels of cospeciation and congruence between phylogenies of parasite and their hosts (Hafner & Nadler, 1990; Lauron et al., 2015; Cruaud & Rasplus, 2016). With this view, host shift would be a rare or exceptional phenomenon (Jaenike, 1990; Via, 1990; Agosta et al., 2010) and the unidirectional specialization would drive species towards an evolutionary dead-end (Moran, 1988; Wiegmann et al., 1993; Kelley & Farrell, 1998). However, empirical evidence has shown that generalist lineages of parasites can be derived from more specialized lineages, and that host switching commonly occurs (Scheffer & Wiegmann, 2000; Janz et al., 2001, Stireman, 2005; Yotoko et al., 2005). The difficulty of reconciling the idea that specialization is always selected with the large evidence showing abundant host shifts is called the "parasite paradox" (Agosta et al., 2010).

An alternative explanation of how the diversity in host range is related to the diversification of organisms is given by the Oscillation Hypothesis (Janz & Nylin, 2008). It proposes that host range changes within different lineages throughout its evolutionary history, with alternate states of specialization (Nylin et al., 2014). When a specialist is exposed to novel resources, it may expand its range to a new host without initial genetic change if it has the capacity to successfully use it and complete its life cycle through a process known as ecological fitting (Janzen, 1985; Agosta et al., 2010). Following this phase of host expansion, the species can subsequently adapt and speciate either in sympatry or parapatry (Janz & Nylin, 2008; Nylin et al., 2014). The ability to use additional hosts can lead to geographic expansion, since the distribution of the original and novel hosts may not be identical. This spatial expansion can eventually lead to local adaptations and reduction of the gene flow, which results in events of specialization and speciation (Janz & Nylin, 2008). The Oscillation Hypothesis was first proposed to explain the pervasive variation in the evolutionary dynamics of the host range in Nymphalidae butterflies (Janz et al., 2001). Its prediction has since gained empirical support from patterns of host association in several other groups (Sedivy et al., 2008; Nilsson et al., 2016; Nylin et al., 2018). The strong relationship between host diversity and parasite richness is also supported by theoretical models (Winkler & Mitter, 2008; Nyman et al., 2010; Araujo et al., 2015; Wang et al., 2017; Braga et al., 2018).

Although the host range can be regarded as a good predictor of species richness in a clade, speciation by ecological factors alone cannot account for all the diversity found in these groups (Janz et al., 2006). Geographical factors are also likely to play a major role in reducing populations' gene flow and promoting speciation (Hawthorne & Via, 2001; Kelley et al., 2000; Servedio, 2015). Hence, diversification processes can hardly be untangled from a spatial context (Mayr, 1963; Servedio & Kirkpatrick 1997; Gavrillets 2004; Kisdi & Prikopil 2011; Rettelbach et al., 2013). Space might influence speciation mainly because of two different processes. Differences in dispersal capacities can limit gene flow, leading to increasing differentiation between the populations, and eventually promoting their reproductive isolation (Wright, 1943; Fitzpatrick et al., 2009) even in the absence of natural selection (Hoelzer et al., 2008; Aguiar et al., 2009). The other aspect is that the geographical occurrence of a parasite determines the potential hosts it can interact with and therefore the set of selective pressures acting on its populations (Thompson, 2005), and vice versa (Slove & Janz, 2001). The increase in host use can be

related to geographical expansion, which in turn affects the chances of local adaptation and new specialization and speciation events (Janz & Nylin, 2008).

Integrating the evolutionary dynamics of host use in a geographical context can thus be an important step in advancing our understanding of how ecological adaptation and spatial gene flow interact on outcomes of species diversity and the evolution of specialization patterns. In this paper, we propose an Individual-Based Model with evolving *in silico* populations of genetically explicit individuals to investigate how selection due to host use and geographic distribution affects speciation dynamics and variation in host range. We characterize the variation in host range along time, during and between events of speciation. By considering that both phenomena (speciation events and host use) emerge from the interaction of lower-level agents, instead of being imposed a priori, we aim to test the prediction that oscillations in host range are an expected outcome of the evolutionary dynamics in diversification processes associated with ecological adaptation in a geographical context. By controlling the influence of these factors, we can evaluate their contribution to speciation likelihood and directions in specialization across evolutionary time.

2 MATERIALS AND METHODS

In this study, we used an Individual-Based Model to investigate the patterns of species richness and dynamics in host use when individuals evolve in a spatial landscape with different hosts. The model is based on the interacting life cycle and dynamics of phytophagous insects and their host plants, but its principles can be extended to other parasite-host and antagonistic systems. The agents represent individuals from a higher trophic level (consumers) that exploit host species from a lower trophic level (hosts). We used the framework developed by Aguiar et al., (2009) to characterize the individuals' genome and the speciation process due to reproductive incompatibility. The model is spatially explicit for both consumer and host distributions. The latter also imposes a selective pressure on the consumer's fitness by trait matching, but the host distribution is not affected by the consumer. A species host range (HR) is defined by the number of different hosts successfully used during each generation. We measured the resulting species richness, frequency, and intensity of oscillation events on host range according to the individual's dispersal capacity and intensity of selection. The modeling approach and these metrics are detailed below.

2.1 MODEL DESCRIPTION

2.1.1 Consumer and host definitions

The model is composed of consumers and hosts distributed in a spatial grid composed of $m \times m$ cells (Fig. 1). Each cell can contain a maximum of one consumer. A consumer is characterized by its genome, its phenotype and its spatial position in the grid (i, j) . The genome of the individual in position (i, j) consists of a binary string of size L equal to 100 that assumes values of 0 or 1. The phenotype $z_{(i,j)}$ is assumed as the sum of all values in its genotype:

$$z_{(i,j)} = \sum_{n=1}^L X_{(i,j)}^n, \quad (1)$$

where $X_{(i,j)}$ is a vector that represents its genome, and n the position of each locus. The consumers' phenotype can range from 0 to L .

We modeled N_H types of hosts, each type of host is defined by its imposed favored phenotype, that are separated by equidistant intervals of value P . Thus, hosts are

represented by a number $h_{(i,j)}$ which corresponds to the favored phenotype that is imposed for the consumer that occupies the cell (i,j) . Unlike consumers, hosts are not individually modeled in terms of the genome and do not evolve over time nor move over space. Then, hosts cover all space, composing a heterogeneous fitness landscape, where each grid cell can assume a value $h_{(i,j)}$, which is constant through time. Moreover, we assumed that the favored phenotype distribution presents a partial degree of spatial autocorrelation, instead of a random distribution on the landscape (Malanson, 1985). This spatial structure implies that neighboring cells have a higher probability of harboring hosts of equal or similar values than more distant cells, thus creating patchiness in the resource distribution (Cliff & Ord, 1973). The spatial autocorrelation structure was generated by adapting a sequential Gaussian simulation algorithm (Goovaerts, 1998; Büchi et al., 2009, see details in Supplementary Material 1).

Space also sets encounters with potential reproductive partners and available hosts. Individuals in one location have a list of adjacent cells that defines their spatial neighborhood (Fig. 1. ii). This spatial neighborhood is defined by the grids inside a circular area with radius R , centered at the consumer position. This neighborhood represents the dispersal capacity of the consumer during its life cycle, and consequently the likelihood of finding a partner and the potential host that it can choose for its offspring.

2.1.2 Dynamics

During each cycle of interactions, each individual chooses a partner to mate with, drawn from its spatial neighborhood (see *Reproduction* subsection). The couple can have a maximum of F offspring that disperses to an unoccupied cell of that spatial neighborhood (see *Dispersion* subsection). Each offspring has a chance to die due to the selection imposed by the host (see *Selection* subsection). After all events, the previous generation is replaced by the new generation and the cycle restarts.

2.1.2.1 Reproduction

Following Aguiar et al., (2009), consumers only reproduce with partners possessing a minimum genetic similarity G . The genetic similarity is calculated by comparing the number of loci in each individual's genome that has the same values. If

individuals have a genetic similarity below the G threshold, they are considered incompatible and do not reproduce. When a compatible partner is found, they recombine their genomes and the resulting offspring inherits 50% of each parent's loci (Fig. 1. iii). Variability is added to the system as each locus of the genome mutates at a mutation rate μ . A species is defined in this model as the set of all individuals that are connected by the genetic possibility of gene flow (Aguiar et al., 2009). Note that this definition of species does not require that all individuals are able to reproduce with all other members of the group.

2.1.2.2 Dispersion

The offspring is placed at a host within the parent spatial neighborhood and is selected according to a preference strategy: The parent randomly probes N_{atp} potential locations within its spatial neighborhood. If all locations are occupied this offspring dies. If more than one location is unoccupied, the offspring is placed at the host that maximizes its fitness. This host search represents a simplified process of host preference widely observed in insect oviposition choice (Thompson, 1988; Nylin et al., 1996), prey choice by a predator (Jobin et al., 2000, Araujo et al., 2020) or host nests by bird parasites (Moksnes & Oskaft, 1995). This mechanism of host preference strategy ensures that the host chosen by the parent is neither random nor necessarily the optimal host for the offspring (since the optimal host may not be probed or even available within the spatial neighborhood), allowing a chance that it attempts to colonize non-optimal hosts. The offspring has a chance to die due to the selection imposed by the host (see *Selection* subsection) and if it does, the cell becomes available for next offsprings.

2.1.2.3 Selection

The survival probability (fitness) for each offspring is calculated according to the distance of its phenotype to the favored phenotype imposed by the host (Fig. 1. iv). The fitness of the individual i , $W_{(i,j)}$, is given by:

$$W_{(i,j)} = \exp\left(-\alpha(z_{(i,j)} - h_{(i,j)})^2\right) \quad (2)$$

where $z_{(i,j)}$ and $h_{(i,j)}$ are respectively the phenotype of the consumer and the favored phenotype imposed by the host, and α defines the intensity of the selective pressure. A

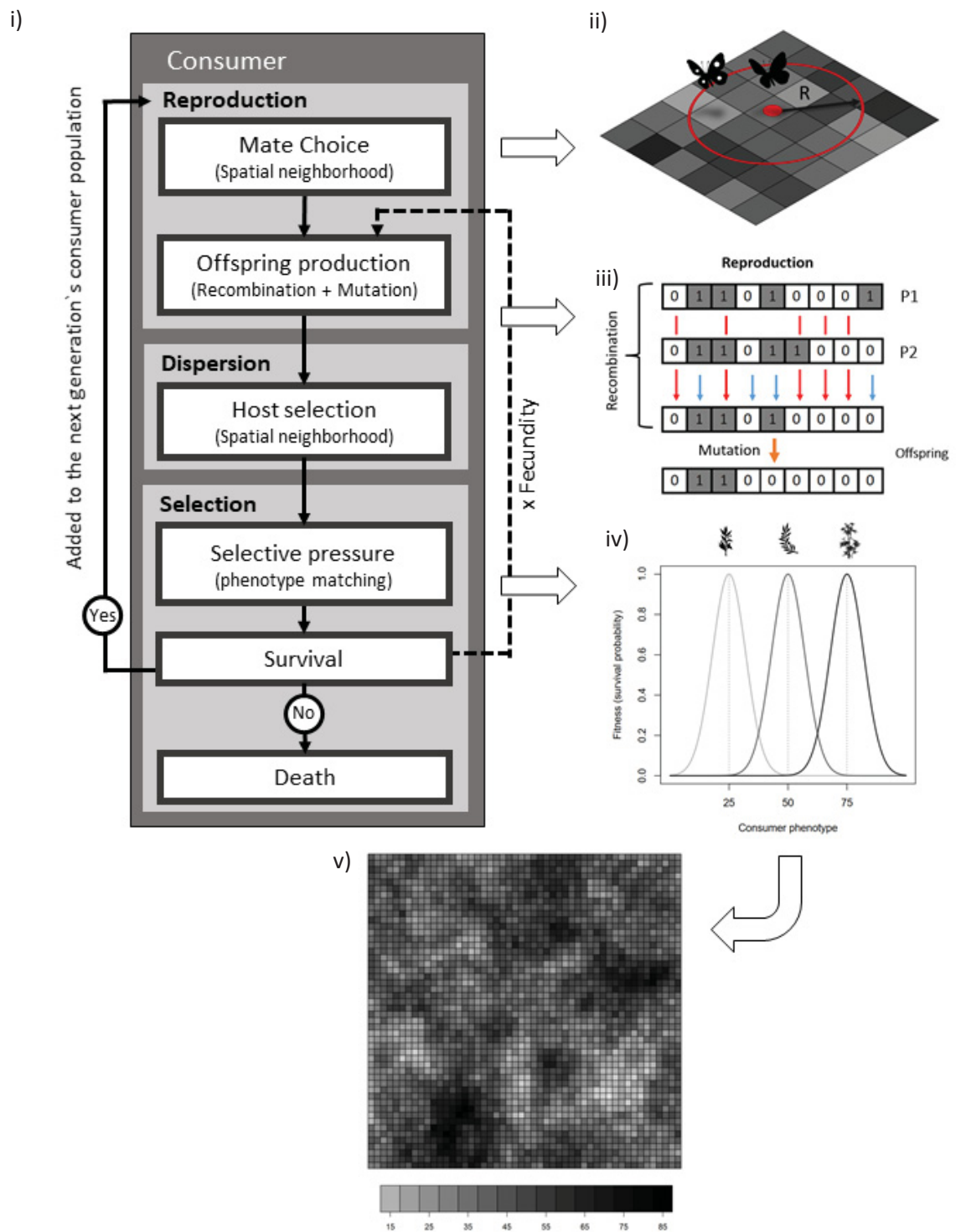


Figure 1. Fluxogram of events and illustration of the model. i) In each generation, consumers chose a compatible mate within its spatial neighborhood of radius R and produce offspring according to its fecundity (F). The parental individual selects a host for its offspring that maximizes its survival probability within its dispersal capacity, also given by R . A selective pressure of intensity α sets the survival probability of each offspring according to its phenotypic fit to the chosen host. The surviving individuals are passed to the next generation, and the cycle restarts. ii) Illustration of a consumer individual and its spatial neighborhood on the grid, where it can find potential mates and hosts for its offspring. iii) Detailed scheme of the reproduction process, in which the offspring inherits half of each parent's genome (P1 and P2) by recombination. Variation

is then added by a mutation in the genome. iv) Example of three hypothetical hosts and consumer fitness according to its phenotype. Each line represents the fitness curve for a different host, which peaks at the favored phenotype that it imposes. v) Spatial landscape showing host distribution, depicting a partial spatial structure for host values. Each color in a cell represents a host and the phenotype value that imposes maximum fitness (survival probability) for the consumer.

high value for the intensity of the selective pressure implies that the consumer's phenotype must closely match the phenotype of the host, while smaller values of selective pressure relax the effect of trait matching on the survival probability of the individual.

2.1.3 Initial conditions

We initialized the simulations with a square of 5 x 5 individuals with identical genomes placed in the center of the grid, each in a different cell, and all their phenotypes equal to $L/2$, half of the genome size. The limited spatial distribution of the consumers at the beginning of the simulations allowed us to evaluate its behavior as if it were equivalent to a scenario of initial colonization followed by geographical expansion.

2.2 ROBUSTNESS AND ANALYSIS

For each simulation, we recorded the total number of consumer species (species richness) and host range (HR) after 1000 generations. In our model, HR is defined as the number of different successfully used hosts by each consumer species in every generation. We consider that a host has been successfully used when at least one consumer individual that attempts to use it survives after the interaction. We also proposed an Oscillation Index to describe the dynamics of variation in host range (described below). We repeated the simulations 10 times for each parameter combination.

We conducted a preliminary analysis of the influence of different parameter combinations (Table 1) on species richness (Supplementary Material 2) and of how the model dynamics depended on the degrees of spatial configuration and number of host searches (Supplementary Material 3). Here we present the effect of the dispersal radius (R) and strength of the selective pressure (α , Table 1). By varying the dispersal radius, we were able to evaluate the role of the spatial distribution of a species in influencing gene flow and the local availability of potential hosts it can interact with. This approach

allowed us to adjust the geographical connectivity of individuals as levels within a continuum, rather than assuming allopatric or sympatric scenarios a priori (Butlin et al., 2008). By changing the strength of the selective pressure, we were able to evaluate the importance of selection due to biotic interactions that can affect the likelihood of speciation and variation in host use. This resulted in a total of 42 parameter combinations of dispersal radius (R) and intensity of selection (α).

Table 1. Parameters combination evaluated for the model. Values in bold were used in the main analysis.

Parameter	Description	Value
N	Number of generations	1000
m	Grid size	50
L	Genome size	100
F	Fecundity	4
μ	Mutation rate	0.001 , 0.003, 0.005
α	Intensity of Selective pressure	2×10^{-1} , 5×10^{-2} , 1.2×10^{-2} , 3.1×10^{-3} , 7.8×10^{-4} , 2×10^{-4} , 4.9×10^{-5} , 0.0 *
R	Dispersal radius	1, 3, 5, 7, 9, 10, 11
G	Genetic threshold	1, 5, 10, 15
N_{atp}	Number of host probing	1, 5, 10
N_H	Number of different favored phenotypes	15
P	Host's favored phenotype interval	5
Ω	Spatial autocorrelation of hosts	0, 5, 10, 15

*These values were set by starting the sequence with $\alpha = 0.2$ and then multiplying each following value by 0.25 in relation to the previous one.

2.3 THE OSCILLATION INDEX

The Oscillation Index evaluates if the consumer host range evolution follows the Oscillation Hypothesis (Janz & Nylin, 2008, Fig. 2) that basically assumes: (i) Host

expansion: a consumer species expands its host range over time up to the point that a speciation event occurs; (ii) Host specialization: the new pair of young consumer species are more specialized (smaller host range) than their common ancestor at the moment just before speciation. We propose an Expansion Index (HEI) and the Host specialization Index (HSI) and then combine both in an Oscillation Index (OI), detailed below.

Let us call t_0 the time that a consumer species arises and t_s the time that a new speciation event arises from this species; that is, the times of the two consecutive nodes of a phylogenetic tree, respectively (Fig. 2). The Host Expansion Index measures the intensity of the host range variation between these two times as:

$$HEI = \frac{HR(t_s) - HR(t_0)}{HR(t_0)}, \quad (3)$$

where $HR(t_s)$ and $HR(t_0)$ means the host range at the time t_s and t_0 , respectively. Observe that HEI is positive if the consumer species expands its host range, it is zero if it does not change and it is negative if the host range decreases between the two events. The index can assume a maximum value of $N_H - 1$, if the lineage starts with just one host and then expands its host range to all hosts in the simulation before speciating. On the other hand, in a case of maximum specialization the index will tend to -1, representing a case in which a lineage starts using all hosts in the simulation and speciates into a lineage that uses just one host.

The Host Specialization Index (HSI) consider only the speciation time and measures the host range variation between the new species and its ancestor species:

$$HSI = 1 - \frac{HR'(t_s)}{HR(t_s)}, \quad (4)$$

where $HR'(t_s)$ means the host range of the new species at the moment when this new species arises and $HR(t_s)$ the host range of the ancestor species at the moment just before speciation (Fig. 3). If the new species keeps the same host range of its ancestor, this index is zero, which means no specialization associated with the speciation. If the new species reduces its host range, this index is positive, and this value tends towards 1 as the host range retraction increases (specialization). This index is never negative once we consider just host range variation associated with the speciation event; new host colonizations can only occur after this event. For each speciation event, we then have two HSI values.

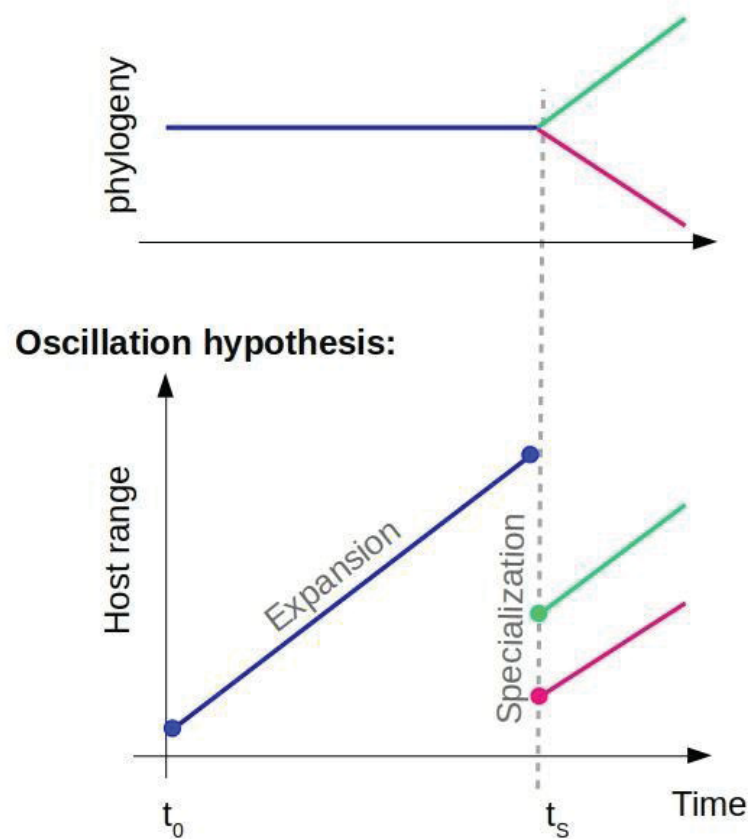


Figure 2. Changes in host range at different evolutionary moments following the Oscillation Hypothesis. The graph above represents the evolutionary history of an ancestral lineage (blue line) that originates two daughter lineages (green and purple lines). The graph below represents each lineage's corresponding host range (HR). The Host Expansion Index measures the direction of changes in host range between a species origin (t_0) and its next speciation event (t_s). Expansion of host range results in a positive HEI, no variation results in $HEI = 0$, and reduction in host range results in a negative HEI. The Host Specialization Index (HSI) for each lineage measures the proportion of hosts that remained after the speciation event. The index is calculated separately for each new lineage since they can have different levels of reduction in host range due to the speciation event. The Oscillation Index summarizes both events (description below). Examples of the measures for the Oscillation Index are shown in Figure 5.

The Oscillation Index (OI) is obtained by multiplying HEI and HSI, which summarizes the variation in host range between speciation events for each new lineage:

$$OI = HEI * HSI. \quad (5)$$

Positive values indicate situations where variation in host range follows the prediction of the Oscillation Hypothesis: events of host expansion of a consumer are followed by a speciation event with specialization (reduction in host range). Zero and negative values indicate situations where oscillations in host range do not occur as predicted by the Oscillation Hypothesis: $OI=0$ when there is either no host expansion or host specialization; $OI<0$ occurs only when the Host Expansion Index is negative; thus

when a consumer species reduces its host range through time without speciation. For each speciation event, we have two OI values with the same HEI value but two possibly different SHI values. The range of values that the OI can assume is very similar to the range of values that the HEI can assume.

In our model, we found a recurring pattern in which the number of individuals in each new lineage was unequal. Thus, one of these lineages maintained a greater number of individuals when compared to the other lineage. This inequality in the number of individuals implied in distinct patterns of variation in host range to each lineage. Therefore, the analysis regarding variations in HR at specialization and oscillation events was done separately for the larger and smaller lineage.

The patterns of variation in host range were evaluated by averaging the index values and the proportion of index values that were positive, negative (when applicable), or equal to zero in each simulation. To describe the overall tendency of the speciation events in the simulations to follow the Oscillation Hypothesis, we calculated the proportion of events that result in positive values of OI for all speciation events occurring in a simulation and also estimated the intensity of oscillations by averaging the OI values greater than zero. In order to understand the effects of intensity of selection and dispersal radius, we then averaged the simulation's proportions and index values for all simulations that had the same parameter combination. Finally, to describe the overall pattern of variation in host range, we calculated the average of proportions and index values for all simulations.

To evaluate how variation in host range is affected by conspicuous geographic expansion, we also applied the index measures for the first speciation event. For most simulations where speciation events occurred, this represents the interval between the initial emergence of a small population and its expansion through most of the spatial landscape.

3 RESULTS

3.1 MODEL DYNAMICS

The model dynamics showed two phases: a pattern of initial geographical expansion of the first species, followed by a second moment consisting of events of fragmentation into multiple species. This pattern occurred for all the evaluated parameter combinations, although the number of speciation events depended on both the dispersal radius and intensity of selection (detailed in the next section). At the beginning of the simulations, all individuals belong to a single population of identical individuals that survives in just one or a small subset of all available hosts. Reproduction leads to an increase in population size and expansion of the geographic distribution (Fig. 3A, upper panel). Gradually, this population acquires increasing phenotype diversity due to the recombination and mutation events (Fig. 3A, lower panel). The species colonize new hosts and expand the range of their host repertoire. A second phase of the model occurs after a few hundred generations, in which the original species starts to fragment into separated lineages (Fig. 3B, upper panel). The new species either persist in the environment and produce new lineages, or they eventually go extinct. After a certain number of generations, the rates of speciation and extinction are balanced so that the number of species approaches an asymptotic value, with small variations due to stochastic fluctuations. The phenotype frequency distribution of each species tends to be unimodal and centered around the host it uses more frequently (Fig. 3B, lower panel), although its shape can vary over time. On a global scale, the whole community uses most of the available host landscape and has a large distribution of global phenotype diversity.

3.2 PATTERNS OF VARIATION IN HOST RANGE AND SPECIES RICHNESS

All scenarios started with the same pattern of variation in host range, regardless of the dispersal radius and intensity of the selective pressure. At first, the initial population was able to use just a small number of hosts. Its increase in abundance and spatial distribution was followed by the inclusion of new hosts, resulting in a significant expansion of its host range (Fig. 4, Table 2). Expansion of host range occurred in all cases before the first speciation event, for every combination of dispersal radius and intensity of selection (Table 2 and Supplementary Material 4). After the first speciation event, the

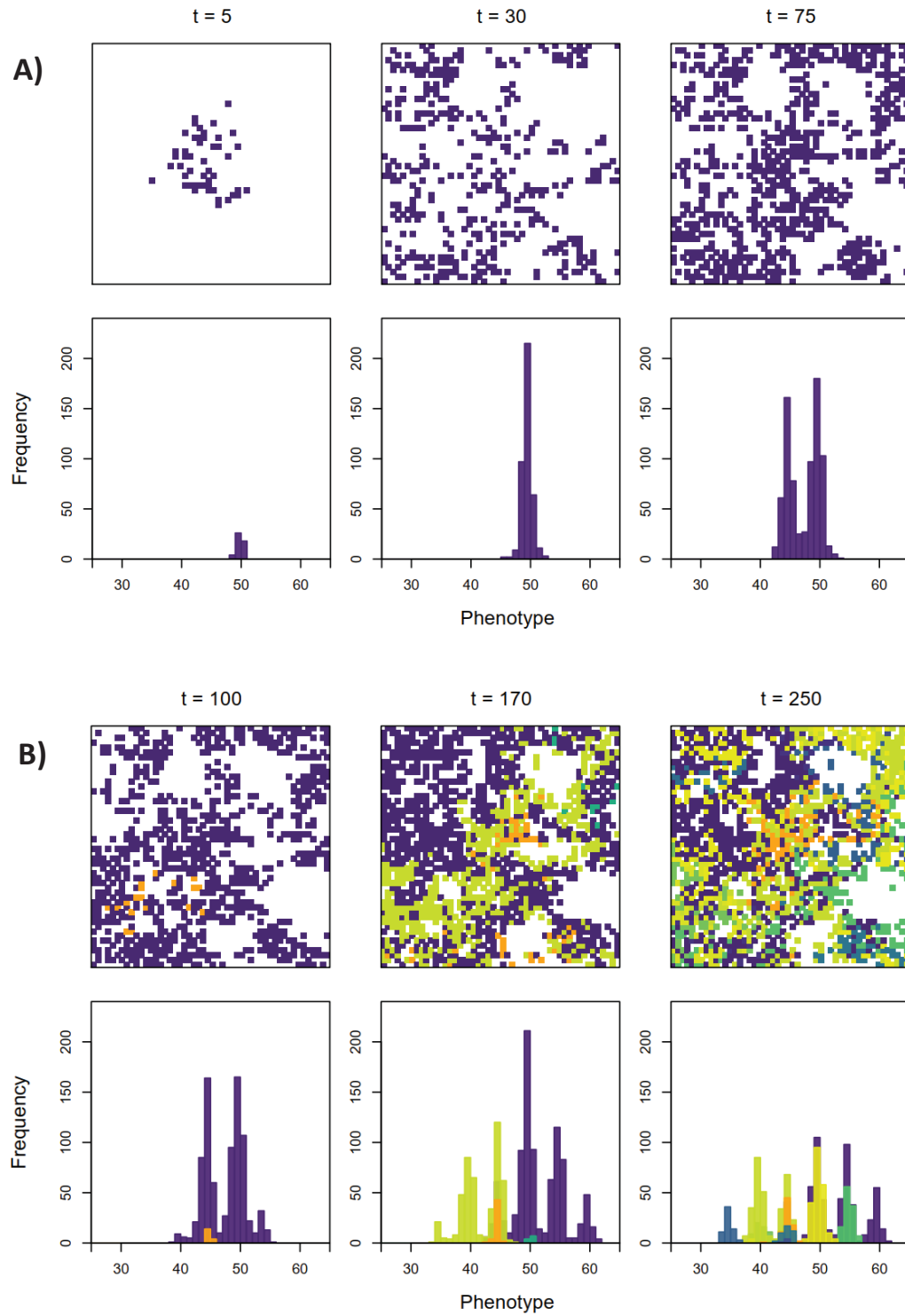


Figure 3. Spatial distribution and phenotype histogram in different generations. For each set, upper panels show the consumer's distribution on the landscape and each dot corresponds to a consumer individual. Lower panels indicate the respective phenotype distribution of species at the same generation of the above figure. Different colors represent different consumer species. Host distribution is not shown but follows A) Phase of geographical expansion of the first species along with an increase in its abundance and phenotypic diversity; B) Second phase of the model, with the fragmentation of the first species into multiple lineages. Parameters for this simulation are: $m = 50$, $L = 100$, $F = 4$, $\mu = 0.001$, $\alpha = 0.2$, $R = 5$, $G = 5$, $N_{atp} = 5$, $\Omega = 5$.

initial lineage was split in two. For the lineage with a greater number of individuals, reductions in its host range occurred only a relatively small number of times (proportion = 0.15, sd = 0.2). The other lineage was composed of a smaller fraction of the individuals and suffered a host range reduction in nearly all occasions (proportion = 0.98, sd = 0.04). This characterizes the first oscillation event of the simulation, in which expansion in host range is followed by a reduction in host range (specialization) at the moment of speciation.

The second phase of the model had a different dynamic, characterized by multiple speciation events associated with patterns of variation in host range (Table 2). The Host Expansion Index showed that host expansions between a species origin and its next bifurcation occurred almost half of the time (proportion = 0.45, sd = 0.05). The events with no variations were less frequent (proportion = 0.33, sd = 0.08), followed by the events with reduction in host range (proportion = 0.22, sd = 0.05). Specialization events followed the same asymmetrical pattern seen in the first speciation event. The lineage that retained most individuals at the moment of speciation had a small likelihood of reducing its host range (proportion = 0.30, sd = 0.08), and on average decreased its host range by one fifth ($HSI_{mean} = 0.22$, sd = 0.09). On the other hand, the lineage with fewer individuals reduced its host range most of the time (proportion = 0.84, sd = 0.11) and reduced its host range by one third at the moment of speciation ($HSI_{mean} = 0.36$, sd = 0.06).

Oscillations in host range emerged along with the speciation events in all scenarios of dispersal radius and selection strength. On average, nearly one-third of events of speciation had positive values of the Oscillation Index, which characterizes expansions followed by specialization (proportion = 0.28, sd = 0.04, Table 2). Events with Oscillation Index equal to zero were frequent (proportion = 0.60, sd = 0.08), as they were characterized either by the absence of host expansion or absence of specialization at the moment of speciation. Events with negative Oscillation Index were less common (proportion = 0.11, sd = 0.05). The frequency of oscillations (i.e. the proportion of events with positive OI) was about 2.5 times higher for species that retained most individuals when compared to the other lineage (proportions = 0.40, sd = 0.06 and 0.16, sd = 0.06 respectively). The intensity of oscillations, given by the mean of positive values of the oscillation index, was also higher for new lineages with fewer individuals ($OI_{mean} = 0.21$, sd = 0.15, $OI > 0$) than the lineages with most individuals ($OI_{mean} = 0.12$, sd = 0.12, $OI > 0$).

The intensity of oscillation was dependent on the intensity of selection and dispersal radius. At the same time, when oscillations did occur in this scenario of strong

selective pressure, they were stronger when compared to simulations with other selection intensities. This can be noticed by higher values of the OI when compared to other simulations (Fig. 5A and 5B). A combination of large dispersal radius and weak or moderate-intensity selection also resulted in higher values for the Oscillation Index for the lineage with fewer individuals, while the other lineage had OI close or equal to zero (Fig. 5A and 5B, the bottom-right region of the graph).

Table 2. Measures for the Expansion, Specialization, and Oscillation indexes. The first three columns show the proportion of events with indexes values greater, equal, and smaller than zero, respectively. The final column shows the mean values for indexes measures greater than zero. Underline values correspond to measures related only to the first speciation event, while the values above correspond to the average value when considering all events in the simulations. Values represent the average \pm standard deviation of all simulations.

Index	Proportion			Mean
	Positive	Equal to zero	Negative	
Expansion	0.45 ± 0.05	0.34 ± 0.08	0.22 ± 0.05	0.51 ± 0.26
	<u>1.0 ± 0.0</u>	<u>0.0 ± 0.0</u>	<u>0.0 ± 0.0</u>	<u>1.35 ± 0.30</u>
Specialization – smaler lineage	0.84 ± 0.11	0.15 ± 0.11	-	0.36 ± 0.06
	<u>0.98 ± 0.04</u>	<u>0.01 ± 0.04</u>	-	<u>0.52 ± 0.12</u>
Specialization – larger lineage	0.30 ± 0.08	0.69 ± 0.08	-	0.22 ± 0.09
	<u>0.15 ± 0.02</u>	<u>0.84 ± 0.20</u>	-	<u>0.12 ± 0.05</u>
Oscillation - both lineages	0.28 ± 0.04	0.60 ± 0.08	0.11 ± 0.05	0.19 ± 0.14
	<u>0.57 ± 0.09</u>	<u>0.42 ± 0.09</u>	<u>0.0 ± 0.0</u>	<u>0.68 ± 0.27</u>
Oscillation – smaller lineage	0.40 ± 0.06	0.42 ± 0.13	0.17 ± 0.07	0.21 ± 0.15
	<u>0.98 ± 0.04</u>	<u>0.01 ± 0.04</u>	<u>0.0 ± 0.0</u>	<u>0.72 ± 0.26</u>
Oscillation - larger lineage	0.16 ± 0.06	0.78 ± 0.07	0.05 ± 0.03	0.12 ± 0.12
	<u>0.15 ± 0.20</u>	<u>0.84 ± 0.20</u>	<u>0.0 ± 0.0</u>	<u>0.16 ± 0.08</u>

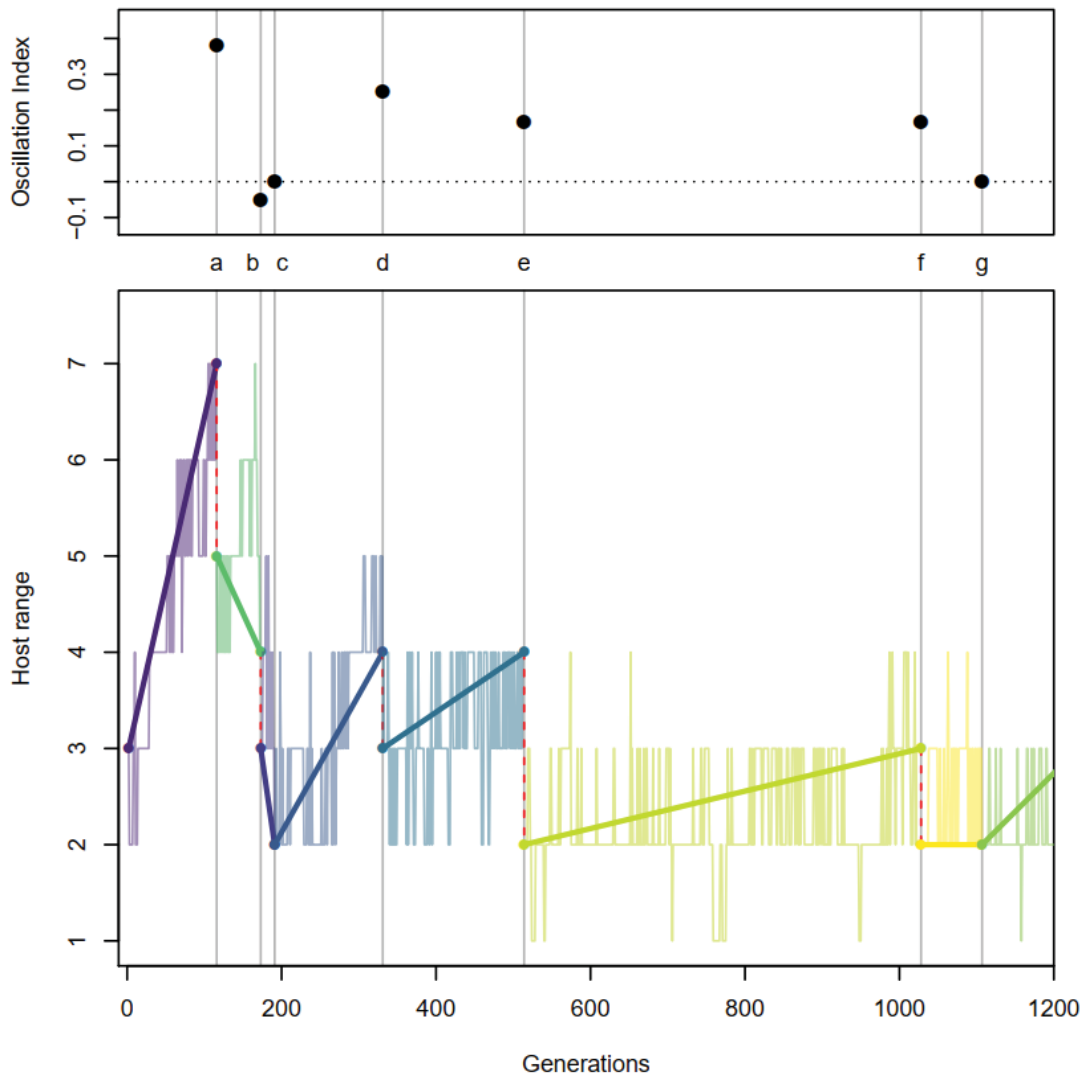


Figure 4. Illustration of the Oscillation Index and host range variation in a simulation. The larger panel shows the variation of host range for different species through time. Each new consumer species is represented by a different color. The straight segments indicate the variation in host range when comparing a lineage's host range between its origin and next speciation events. The red dashed line indicates the decrease in host range following the speciation event. The light lines indicate the host range of each lineage at every generation. Observe that consumers are constantly exploring new hosts and not all new colonizations are maintained over time. In the above panel, we show the Oscillation Index (OI) corresponding to the time of the speciation event. Although each speciation event results in two species, in this illustration, we considered only one in order to not overlap the multiple lines of different lineages. Events *a*, *d*, *e*, and *f* had expansion on host range followed by specialization, hence they have positive values for the OI. Events *c* and *g* had either no specialization or expansion on host range, so their OI is zero. Event *b* had a decrease in host range followed by specialization during speciation, so its OI is negative. Values for the OI are *a* = 0.38; *b* = -0.05; *c* = 0.0; *d* = 0.25; *e* = 0.16; *f* = 0.16; *g* = 0.0.

The species richness of each simulation was strongly related to the length of the dispersal radius and strength of the selective pressure (Fig. 5C). Total species richness increased with a smaller dispersal radius and stronger selective pressure. An exception of this pattern is found for the simulations with the strongest selective pressure that

resulted in small richness or extinction of all individuals. As the consumer's phenotype and their host require a strong match for the offspring to survive under this scenario, individuals have lower performance and the overall abundance is also smaller. The smaller number of individuals in the whole population restricts the potential number of species when compared to a scenario where the system is closer to its capacity of individuals.

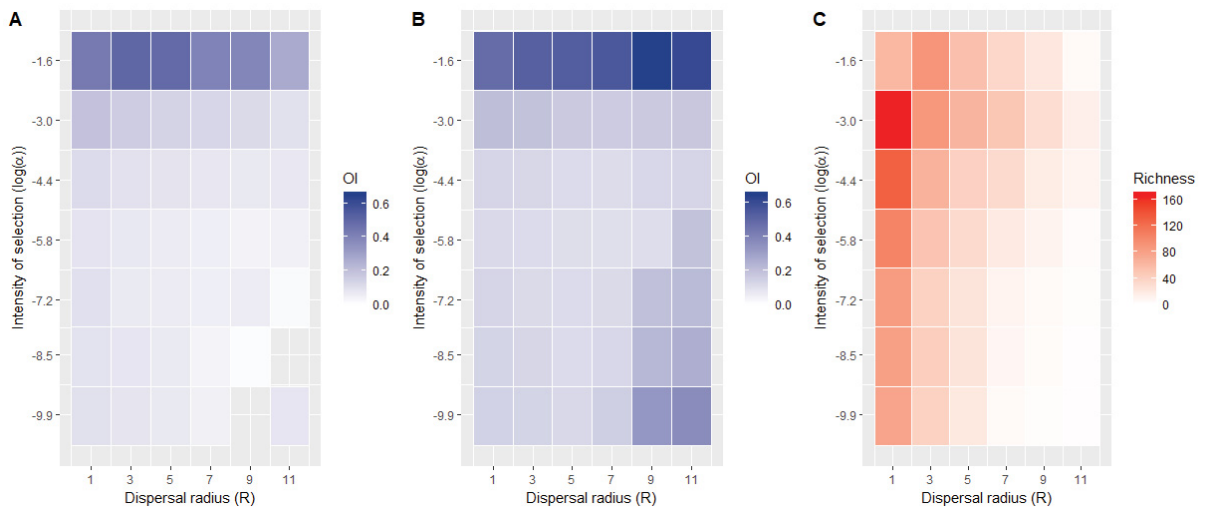


Figure 5. The dependency of oscillation and species richness on interaction strength and dispersion radius. Graphs A and B show the Mean Oscillation Index (OI) for the lineages with most and fewer individuals after speciation, respectively. In both cases, the intensity of oscillation was stronger in the simulations with the highest intensity of selection ($\alpha = 0.2$). C. Species richness.

4 DISCUSSION

In our model, we investigate the expected dynamics for species diversification associated with the evolution of the host range in a spatial context. Our main results show that oscillations in host range are an inherent process of evolutionary dynamics, as it emerged in all scenarios for every dispersal radius and intensity of selection. Throughout the diversification process many lineages repeatedly faced phases of expansion and reduction on its host range, in accordance with predictions of the Oscillation Hypothesis (Janz & Nylin, 2008). Speciation events were preceded by an expansion in host range nearly half of the times, while the species bifurcation led to specialization in one or both lineages. Speciation occurred when the accumulation of genetic differentiation in a population generated groups of reproductively isolated individuals (Aguiar et al., 2009; Aguiar et al., 2017). A stronger intensity of selection and smaller dispersal radius favored an increase in the resulting species diversity. These results suggest that oscillations in host range, rather than ever-increasing specialization, play a fundamental role in species diversification.

At the first stage of the simulations, the initial species expanded its geographical distribution, and this expansion was always associated with an expansion of its host range. When the selection is weak, the colonization of different hosts happens basically as a consequence of the increasing use of space. However, the initial species was able to gradually expand its host range even under intense selection pressure on resource use. This situation is a typical description of the Parasite Paradox (Agosta et al., 2010): if the consumer is suffering high interaction selection and, therefore, needs to specialize on its host in order to perform well on it, how can the host range expand? Our simulations showed that individuals are constantly exploring the boundaries of their fitness curve, and by exposing themselves to selection on marginal hosts they expand their capacity (Fig. 4). During a lineage lifetime, hosts were continuously being lost and colonized by a species. Given enough opportunity and time, new hosts can be incorporated into the consumer's host repertoire (Araujo et al., 2015). This dynamic agrees with the empirical evidence that phytophagous insects and parasites can quickly shift to new related hosts in observable time (Tabashnik, 1983; Singer et al., 1993; Agrawal, 2000; Magalhães et al., 2007). According to Janzen (1985), new hosts can be incorporated into a species repertoire without the requirement of evolutionary innovations. This process is called "ecological fitting" and occurs when traits already possessed by an organism allow it to

survive and persist on resources outside its original range (Agosta & Klemens, 2008; Agosta et al., 2010). This region of potential positive fitness represents the “sloppy fitness space” (Agosta & Klemens, 2008) that can be successfully used given the opportunity (Araujo et al., 2015). In the model, the extent of the “sloppy fitness space” is related to the intensity of the selective pressure. With time, recombination and mutation events increased the phenotypic diversity of the population, allowing it to constantly expand its host range to more distant hosts. Gradually, the increase in the phenotypic variability associated with an increase in the host repertoire allowed the initial species to become a generalist, as a single species was able to use most of the hosts in the system. This phase of geographical and host expansion however represented only a transient state in the simulations, as the initial species quickly broke down into multiple species.

Speciation events were associated with specialization (reduction in host range) in a high number of events. This pattern was also found on another spatially explicit model that explored variations on diet breadth (similar to our host range), although some assumptions and results differ (Forister & Jenkins, 2017). The modeling approach of Forister & Jenkins (2017) focus on expected levels of specialization on the absence of selection, speciation is modeled phenomenologically (Kopp, 2010), and expansion on diet breadth between speciation events are not investigated. A pattern that was not anticipated in our model that emerged from the model was that specialization was uneven and associated with the relative abundance of each new lineage. The phenotype distribution of a consumer species follows a multimodal distribution where each peak corresponds to the favored phenotype imposed by each different host. When the consumer species fragmented in two, the lineage that retained most individuals seldom specialized, which means that a speciation event generally did not break the phenotype distribution of this new species (Fig. 3B). On the other hand, the lineage with fewer individuals frequently contracted its host range at the moment of speciation. This host range reduction was a direct consequence of population fragmentation, as individuals of this new species represent a non-random subset of the incipient species. This division is followed by a loss of genetic and phenotypic diversity when compared to the ancestral species. Thus, specialization emerged as a consequence of the speciation (Patten, 2008), which resulted in asymmetric variation in the host range. Models that consider species as composed of a set of individuals with explicit traits also demonstrate that inheritance of quantitative traits can be asymmetric (Duchen et al., 2019), and here we extend this pattern to asymmetrical variation in host range due to speciation. Asymmetries in host range

variation have already been proposed as a component of specialization-by-drift models based on empirical findings from scale insects (Hardy et al., 2016), and also on neutral models of the evolution of dieth breadth (Forister & Jenkins, 2017). Since this pattern emerged for all selective pressure intensities, our model suggests asymmetry can be produced by speciation driven by either non-adaptive or adaptive forces.

Following the first speciation event, the system converged to a state where multiple species were constantly emerging, along with variation in the host range of these lineages. Expansions of the host range between a species origin and its next speciation event were common outcomes of this phase. The high frequency of events in which the host range expanded suggests a tendency for the lineages to increase its repertoire before speciating again. Expansions of the host range were associated with increased abundance, which in turn increases the overall genotypic variability within the population. The variability in the population associated with dispersal limitation favored the likelihood of speciation events. This dynamic aligns with predictions of the Oscillation Hypothesis, in which host expansions set the stage for posterior processes of increasing genetic differentiation and separation of lineages (Janz & Nylin, 2008). At the same time, about one-third of speciation events were not preceded by changes in the host range, which shows that speciation also occurred without the requirement of host expansion. It is expected that not every speciation event is absolutely associated with host expansion (Janz et al., 2006), and previous models show that differentiation can occur solely due to assortative mating caused by spatial and genetic differences (Aguilar et al., 2009). The second part of our hypothesis predicts that clades that have undergone the oscillations outlined above should be more species-rich compared to clades that have remained specialized on the same host (Janz et al., 2006), which will be addressed in future research.

When comparing the dynamics of the model between the initial phase of geographical expansion to the second phase of the model, the coexistence of multiple species resulted in a different dynamics for both diversification and evolution of host range. The species diversity evolved to a near-equilibrium stage, where it fluctuated around similar values. This equilibrium in diversity emerges in the model as a consequence of spatial limits in the number of individuals that can exist at the same time (MacArthur, 1969; Rosenzweig, 1975). New species are continually formed at a similar rate in which other species became extinct. A large proportion of these newly formed species also did not persist many generations, corresponding to a high frequency of

ephemeral species (Rosenblum et al., 2012). Also, the possibility of each species to use other resources and increase its size was partially limited by competition with the other species (Price & Kirkpatrick, 2009). Hence, although host expansions still occurred during this phase, it had a lower amplitude when compared to the host expansion of the first species.

Oscillations in host range were a recurrent outcome of variation in host range when associated with the diversification process and appeared for all the evaluated levels of selection intensity and dispersal capacity. We highlight that oscillations occurred in nearly all events associated with the initial geographical expansion for at least one of the lineages. This outcome agrees with the expectation from the Oscillation Hypothesis, in which the geographic expansion followed by speciation and specialization produces oscillations (Janz & Nylin, 2008). In our simulations, the increase in geographic range led inevitably to the colonization of new hosts, and the first speciation event led to increased specialization (smaller host range) at least in the less abundant lineage. In the second phase of the model, given by the coexistence of multiple species and a greater limitation of geographical expansion due to the saturation of available space, oscillations still emerged with frequency throughout the multiple speciation events. These findings contrast with the expectation that increasing diversity must be driven by continuous specialization of the lineages (Futuyma & Moreno, 1988; Agosta et al., 2010). In fact, continuous specializations, measured by negative Oscillation Index (or negative Expansion Index) in our model, were the least frequent event that emerged in simulations. It is interesting to note that oscillations occurred even in the scenarios with the highest intensity of selection, which indicates the capacity of species to oscillate their host ranges even when selection imposes the necessity of high adaptation to a host to allow its survival. In order for multiple specialization events to occur along with the speciation events, host expansions must keep adding “fuel” for this process to persist (Janz et al., 2006). Also, the lineages with smaller abundance after speciation, that most frequently specialized after the division, had a higher probability of expanding its host range and oscillate during its next speciation event than its sister lineage. On the other hand, the lineages with most individuals had a smaller chance of either specialize after the division or expanding its host range until its next speciation event and thus contributed mostly to the great frequency of speciation events with no oscillation.

Although the proportion of variations in host range was not so strongly affected by different combinations of dispersal radius and intensity of selection, they strongly

affected the resulting species diversity. Increasing the intensity of selection and decreasing the dispersal capacity resulted in a higher number of species. This process occurred because of two mechanisms. The wide geographic distribution limits the genetic flow even in the absence of barriers, due to limits in the dispersal capacity of organisms. Multiple species can arise solely due to spatial restrictions (Aguiar et al., 2009), as the whole mixing of a widely distributed population is unstable given dispersal limitations (Martins et al., 2013). The second consequence of geographical expansion is related to the expansion of host use. Increasing resource variability presents different selective pressures on individuals, and induces divergent selection (Via et al., 2000; Hendry et al., 2002; Hartmann et al., 2018). Selective pressure imposed by different hosts favored the formation of distinct phenotypic clusters, and hence genetic differentiation within the populations (Rice & Hostert, 1993; Saint-Laurent et al., 2003). The genetic diversity resulting from the adaptation of individuals to different resources (or fitness peaks) led to the reproductive isolation of populations and the formation of distinct species (Dieckmann & Doebeli, 1999; Berlocher & Feder, 2002; Drés & Mallet, 2002). Although in our model both mechanisms were able to separately induce speciation events, their combined effect resulted in increased richness when compared to their effects alone.

Our modeling approach sought to investigate the patterns of variation in host range associated with species diversification that emerge considering both a spatial context and selection imposed by a variety of resources. A few important assumptions were made in order to minimize the level of complexity of the model. First, the favored phenotype imposed by the hosts was unidimensional and equidistantly distributed along the fitness landscape. In natural systems, we expect the resource space is given by the host to be heterogeneous (Nyman, 2010) and composed of multiple dimensions (Fordyce et al., 2016). The hosts' abundance and spatial distribution can also be affected by the interaction with the consumer (Maron & Crone, 2006), and selective pressure exerted by the consumer on the host population can shift the favored phenotype as a consequence of an arms-race dynamics (Erich & Raven, 1964; Hiltunen & Becks, 2014). Also, both dispersal capacity and selection strength are not equal nor constant within all species (Steven et al., 2010; Benkman, 2013; Sweet & Johnson, 2018). Finally, the resource landscape can present different levels of resource availability and connectivity (de la Penã, 2011). For instance, isolated patches can be used to investigate the relationship between allopatric modes of speciation and the evolution of host range (Coyne & Orr, 2004). By examining the outcomes of the model with the simplifying assumptions, we can

have a baseline of expectations for variations in host range and species diversification in a geographical context. This general framework can be useful when assessing and comparing the results after the inclusion of additional and more particular assumptions.

In conclusion, our model was able to simultaneously incorporate the effects of species dispersal and selective pressure by different hosts on diversification processes of species. Although speciation can occur due to each of these processes alone, here we show that they interact to produce even higher diversity when acting combined. Also, the variation in host use is consistent with the predictions of the Oscillation Hypothesis, as events of expansion of host range followed by specialization and speciation represent the basic elements predicted by the Oscillation Hypothesis (Niklas & Janz, 2007). In our simulations, phases of expansion and contraction of host range emerged from the interaction between processes of sexual reproduction of individuals and adaptation to a heterogeneous fitness landscape in a spatial context. We hope that by integrating different but non-exclusive hypotheses on diversification patterns, we can better recreate a more complete picture of how these processes act mutually to explain species biodiversity.

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SUPPLEMENTARY MATERIAL 1

The spatial distribution of hosts was generated by applying a modified sequential Gaussian simulation algorithm. Given an autocorrelation range (Ω), the algorithm sets the above distance between two cells that will have a correlation lower than 0.05. Values distribution was implemented with the *gstat* package (Pebesma, 2004) by the R software v.3.5.2 (R Core Team, 2003). Since the algorithm generates continuous values with mean zero and standard deviation of one, we transformed them into values that correspond to the fitness peaks imposed by the hosts. The mean was adjusted to equal to half of the genome size and we set equidistant breaks by a distance of 5 between 0 and 100. The continuous values were then rounded to the closest and smaller break, creating a distribution of discrete values.

To evaluate the spatial structure generated by the modified algorithm, we measured the spatial autocorrelation range with the input Ω . In spatial statistics, semivariance is the degree of spatial dependence of values in a spatial landscape (Cressie, 1993). The variogram describes how semivariance changes according to the distance between two values, and it is usually described by three parameters. The nugget is the first semivariance value at the horizontal axis origin, the sill is the theoretical limit of the variogram when tending to infinite distances, and range is the distance in which values will show no variation in its spatial dependence (Fig. S1). To analyze the actual range produced by our algorithm, we fitted an exponential variogram model. We found that although algorithms set with $\Omega = 0, 5$ and 10 had range values centered around the spatial autocorrelation values intended for the distribution, there was significant variation around these values. Also, spatial distribution with $\Omega = 15$ did not increase the range when compared to $\Omega = 10$, showing a limitation in the maximum amount of spatial autocorrelation that can be generated by this algorithm (Fig. S2).

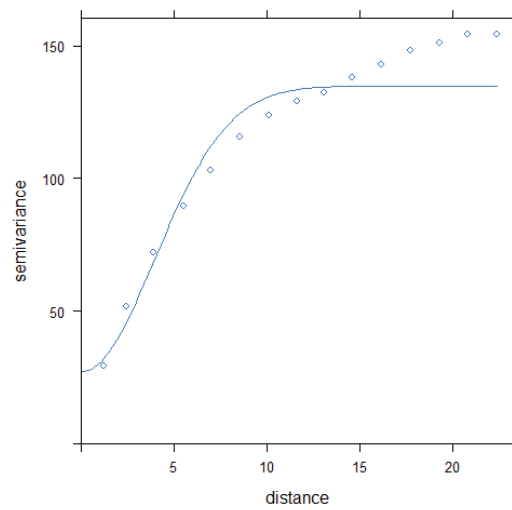


Figure S1. Example of a variogram fitted with an exponential variogram model.

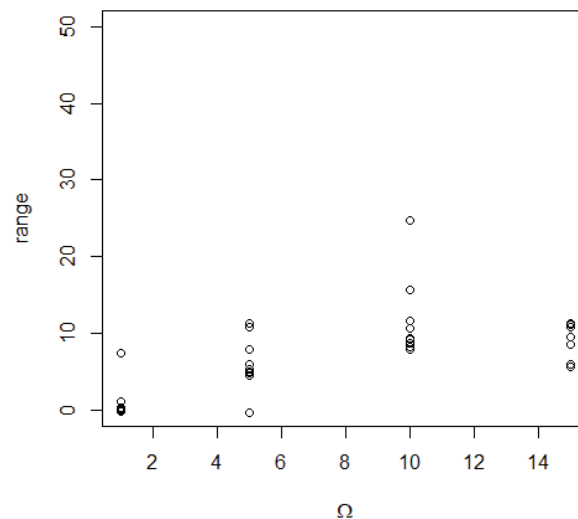


Figure S2. Relationship between range and input autocorrelation (Ω) set for the modified sequential Gaussian simulation algorithm.

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SUPPLEMENTARY MATERIAL 2

Robustness analysis on species richness for different parameter combinations of N_{atp} , μ , α , G and R . All other parameters for these simulations were: $m = 50$, $L = 100$, $F = 4$, and $\Omega = 5$. Each figure shows a different value of N_{atp} , while varying the other parameters. Note that the overall pattern of species richness is very similar when considering $N_{atp} = 5$ and $N_{atp} = 10$.

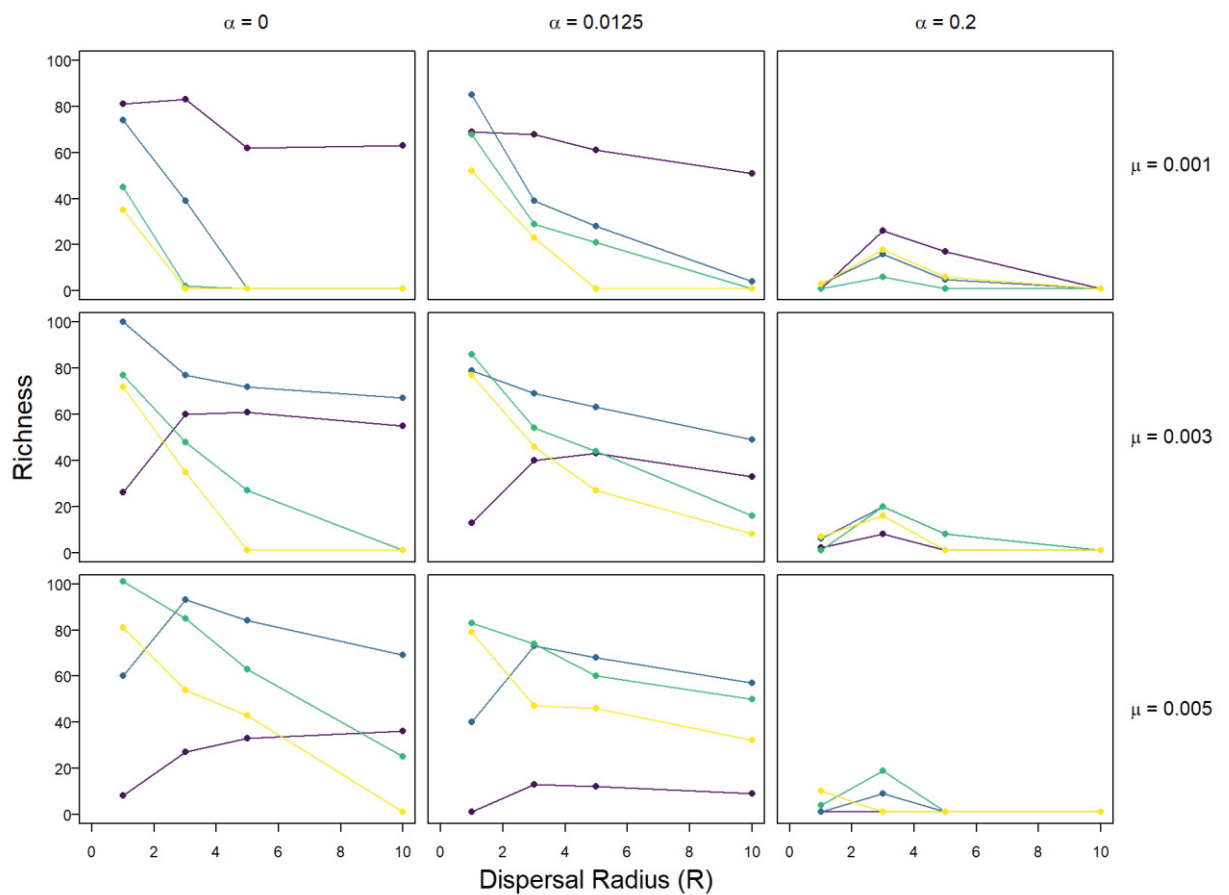


Figure S3. Species richness for different combinations of dispersal radius (R), mutation rate (μ), intensity of selection (α) and genetic threshold (G) when the number of host search (N_{atp}) = 1. Purple line: $G = 1$; Blue line: $G = 5$; Green line: $G = 10$; Yellow line: $G = 15$.

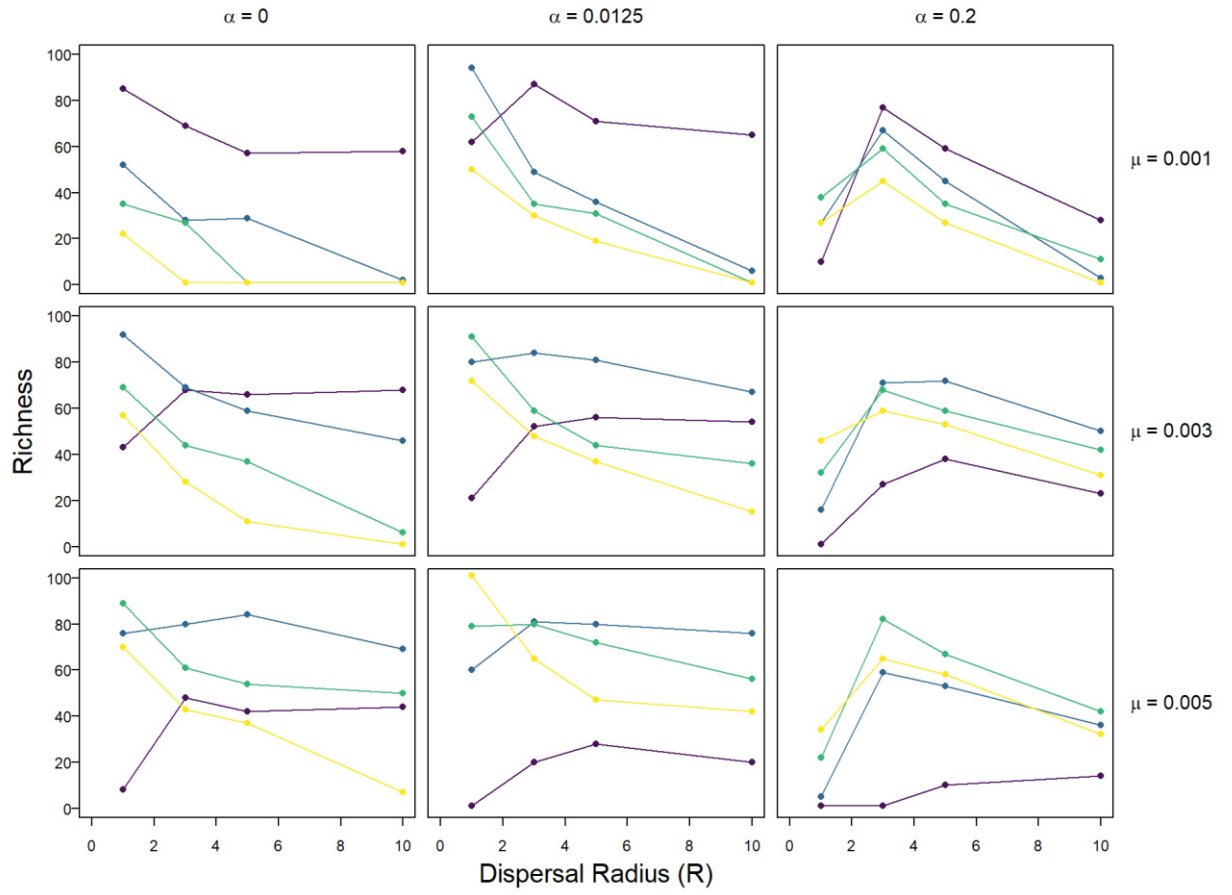


Figure S4. Species richness for different combinations of dispersal radius (R), mutation rate (μ), intensity of selection (α) and genetic threshold (G) when the number of host search (N_{atp}) = 5. Purple line: $G = 1$; Blue line: $G = 5$; Green line: $G = 10$; Yellow line: $G = 15$.

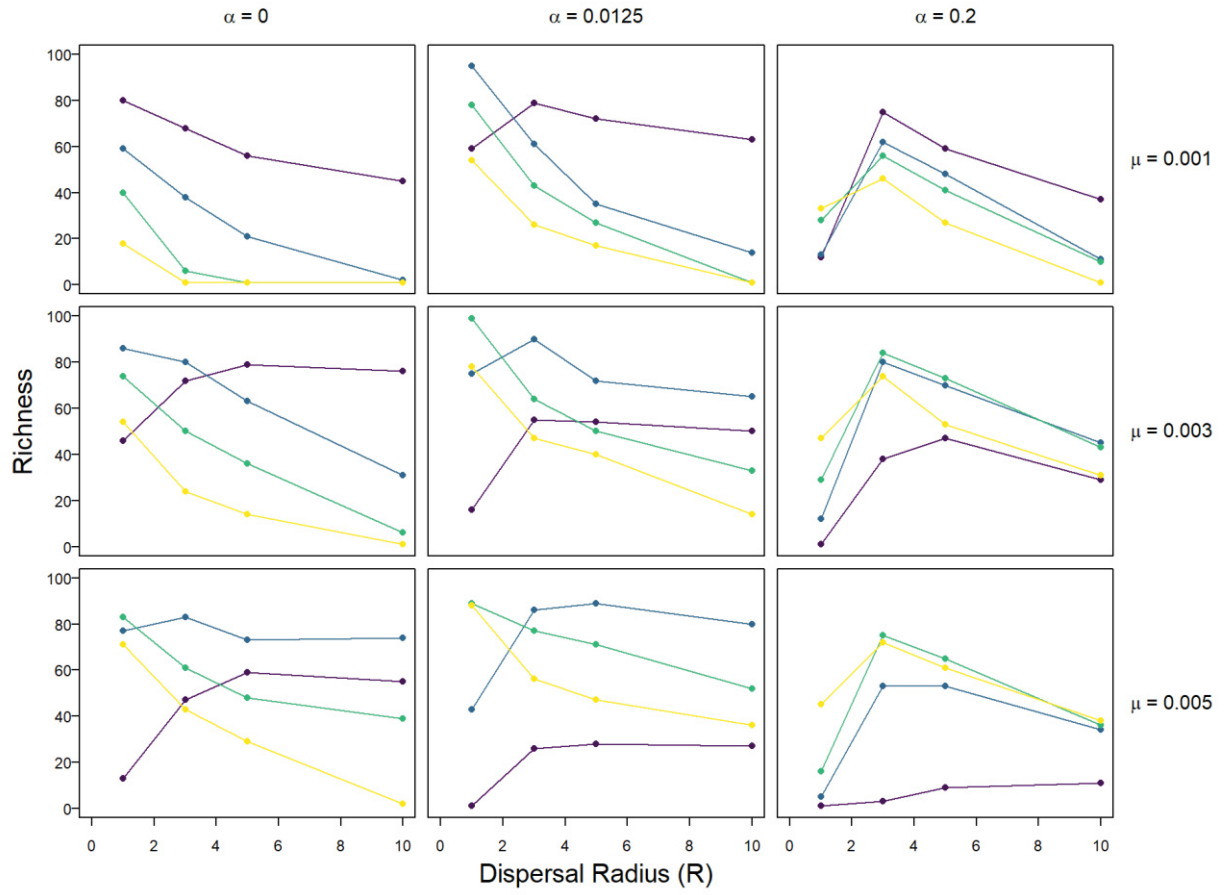


Figure S5. Species richness for different combinations of dispersal radius (R), mutation rate (μ), intensity of selection (α) and genetic threshold (G) when the number of host search (N_{atp}) = 10. Purple line: $G = 1$; Blue line: $G = 5$; Green line: $G = 10$; Yellow line: $G = 15$.

SUPPLEMENTARY MATERIAL 3

The preliminary analysis showed that there was no significant variation in the final species richness when varying the number of host searches on host selection or setting different values of spatial autocorrelation of hosts when it is not random ($\Omega \neq 0$). Also, when more than one species emerged in the simulations, richness increased after a transient period and reached relatively stable values for the same parameter combinations.

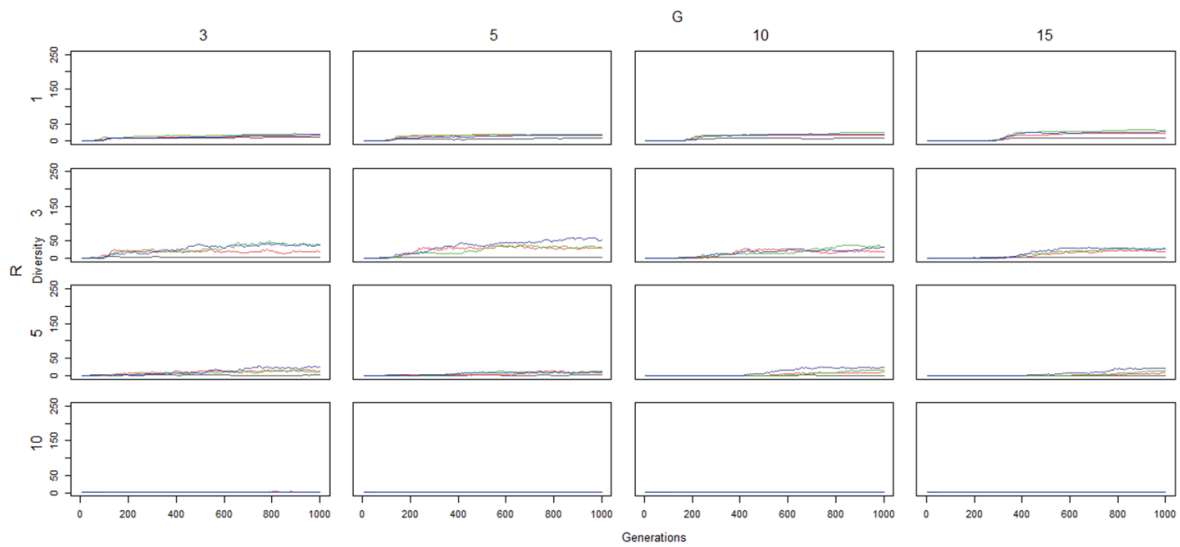


Figure. S6. Species richness through time on simulations with different combinations of dispersal radius (R), genetic threshold (G) on the scenario with random landscape ($\Omega = 0$). Black line: random host probing; Colored lines: preference on host probing, with the following number of search attempts: red line: 3, green line: 5; blue line: 10. Other parameters were: $m = 50$, $L = 100$, $F = 4$, $\mu = 0.001$, $\alpha = 0.2$.

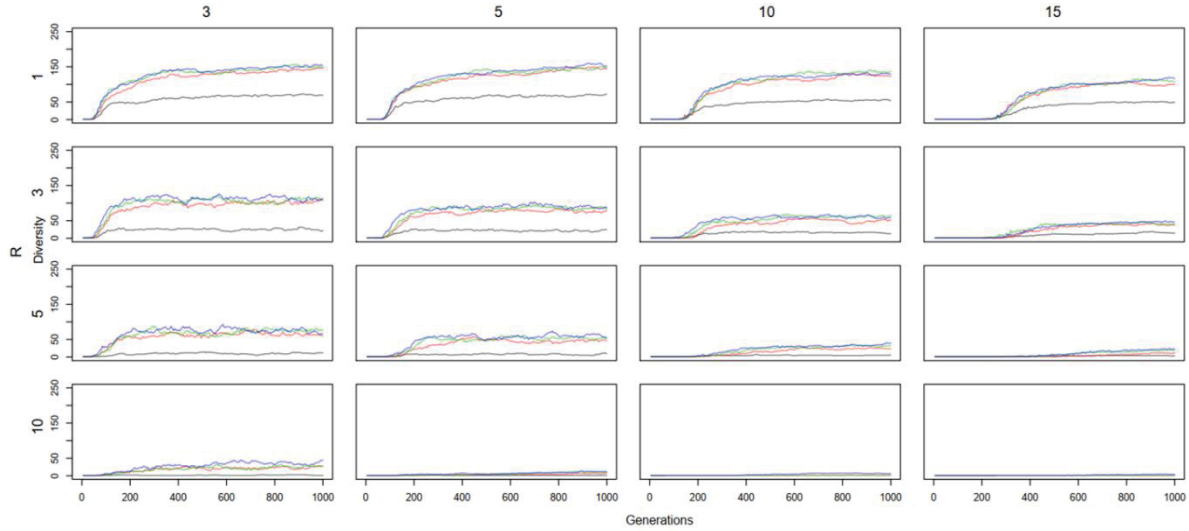


Figure. S7. Species richness through time on simulations with different combinations of dispersal radius (R), genetic threshold (G) on the scenario with random landscape ($\Omega = 5$). Black line: random host probing; Colored lines: preference on host probing, with the following number of search attempts: red line: 3, green line: 5; blue line: 10. Other parameters were: $m = 50$, $L = 100$, $F = 4$, $\mu = 0.001$, $\alpha = 0.2$.

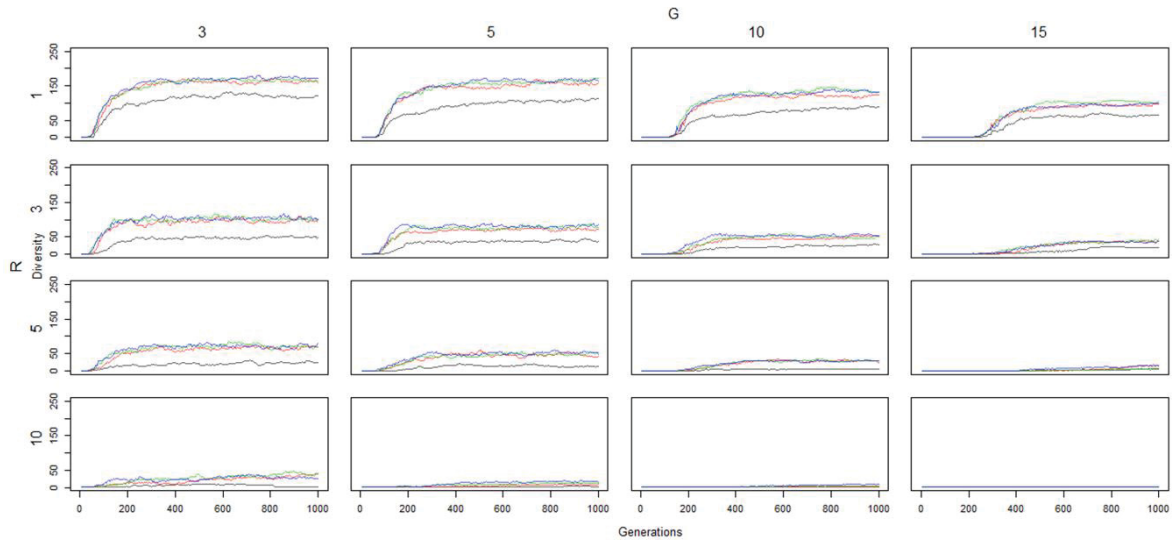


Figure. S8. Species richness through time on simulations with different combinations of dispersal radius (R), genetic threshold (G) on the scenario with random landscape ($\Omega = 10$). Black line: random host probing; Colored lines: preference on host probing, with the following number of search attempts: red line: 3, green line: 5; blue line: 10. Other parameters were: $m = 50$, $L = 100$, $F = 4$, $\mu = 0.001$, $\alpha = 0.2$.

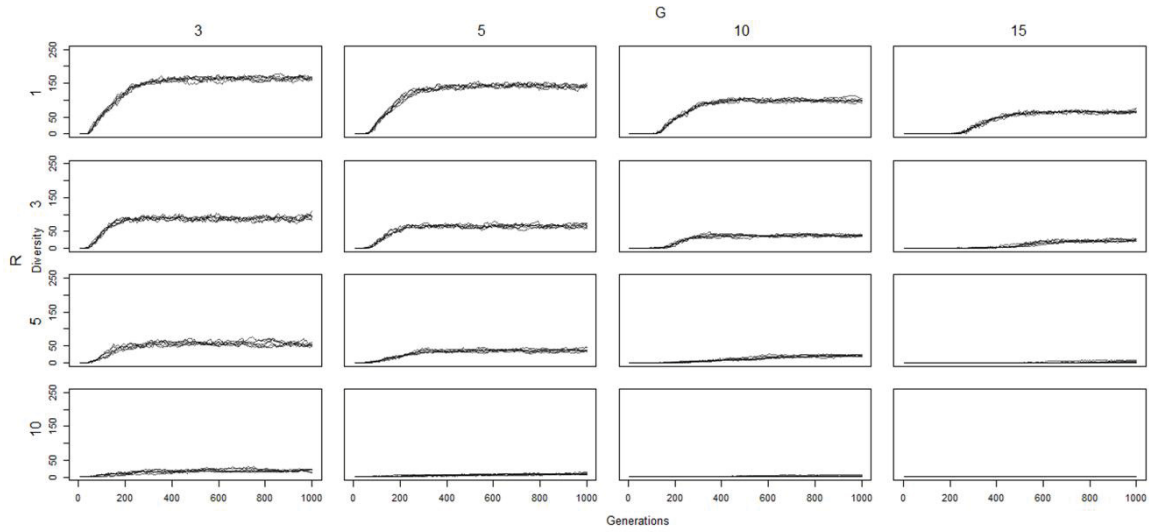


Fig. S9. Species richness through time on simulations with different combinations of dispersal radius (R), genetic threshold (G) on the scenario with random landscape ($\Omega = 25$). Black line: random host probing; Colored lines: preference on host probing, with the following number of search attempts: red line: 3, green line: 5; blue line: 10. Other parameters were: $m = 50$, $L = 100$, $F = 4$, $\mu = 0.001$, $\alpha = 0.2$.

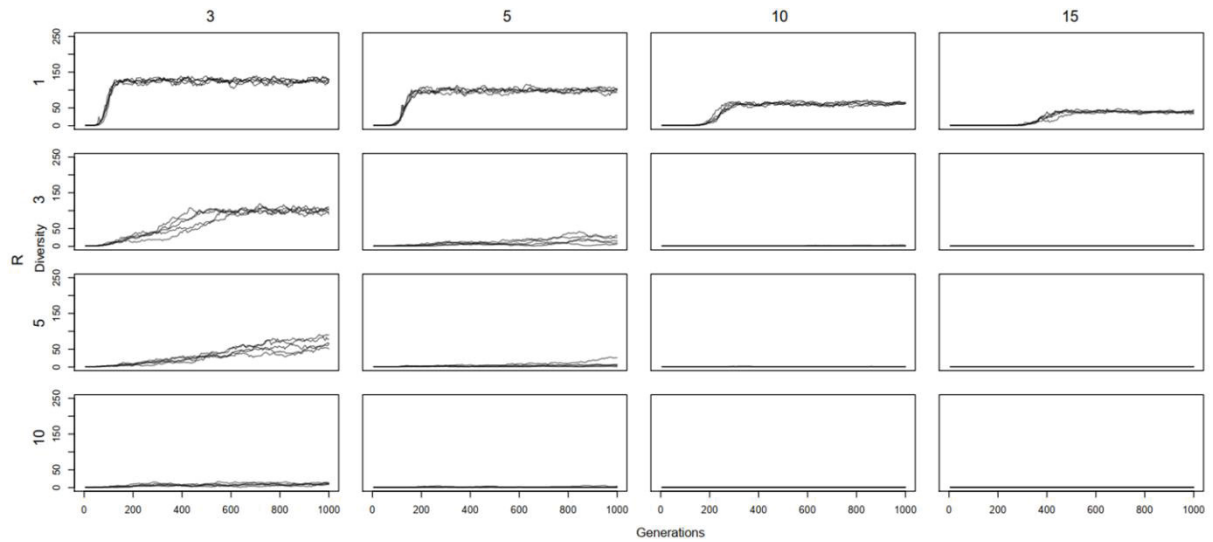


Figure. S10. Species richness through time on simulations with different combinations of dispersal radius (R), genetic threshold (G) on the scenario with neutral selection ($\alpha = 0$). Dark lines represent different number of search attempts ($N_{atp} = 1, 3, 5, 10$). Other parameters were: $m = 50$, $L = 100$, $F = 4$, $\mu = 0.001$, $\alpha = 0.2$.

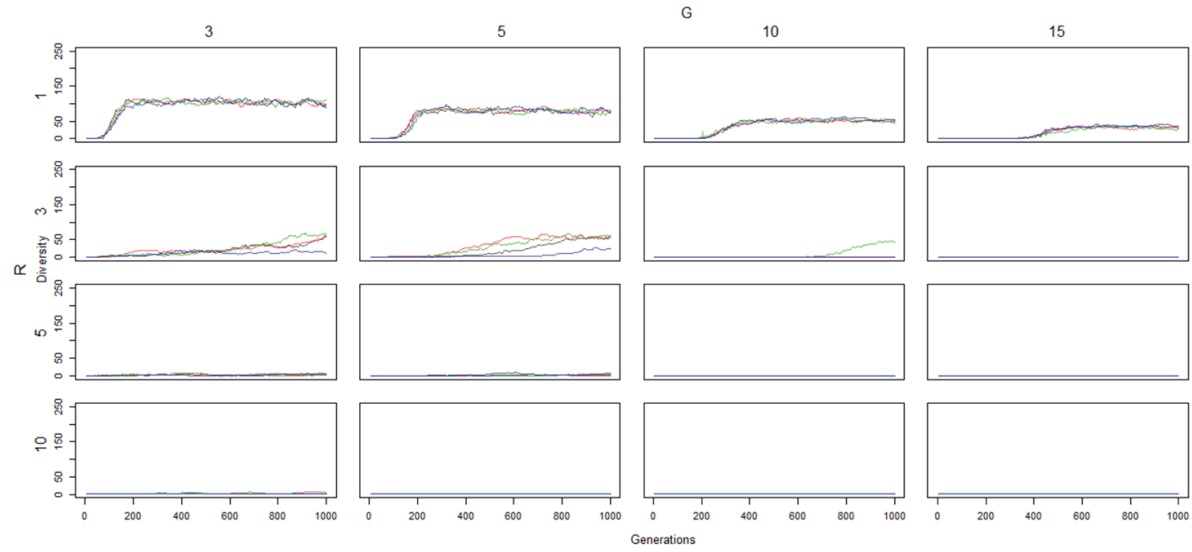


Figure. S11. Species richness through time on simulations with different combinations of dispersal radius (R), genetic threshold (G) on the scenario where all resources had the same value ($j = 50$). Black line: random host probing; Colored lines: preference on host probing, with the following number of search attempts: red line: 3, green line: 5; blue line: 10. Other parameters were: $m = 50$, $L = 100$, $F = 4$, $\mu = 0.001$, $\alpha = 0.2$.

SUPPLEMENTARY MATERIAL 4

Here we show the index measures for the first speciation event for different parameter combinations of R and α . For each parameter combination, we show the average measure for 10 repetitions.

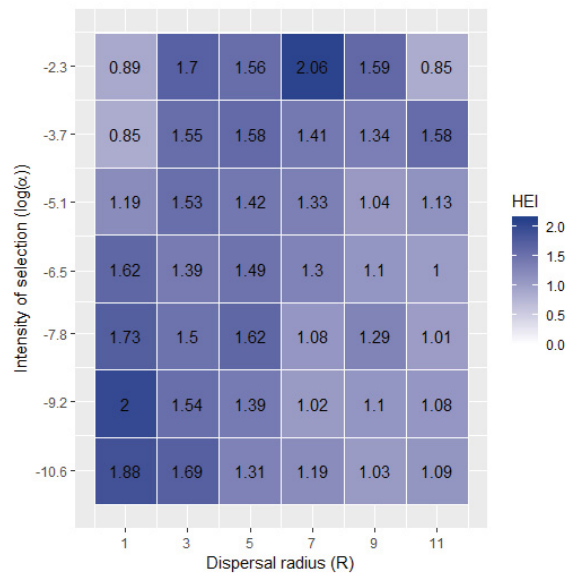


Figure S12. Host Expansion Index for the first speciation event for different values of dispersal radius (R) and intensity of selection (α).

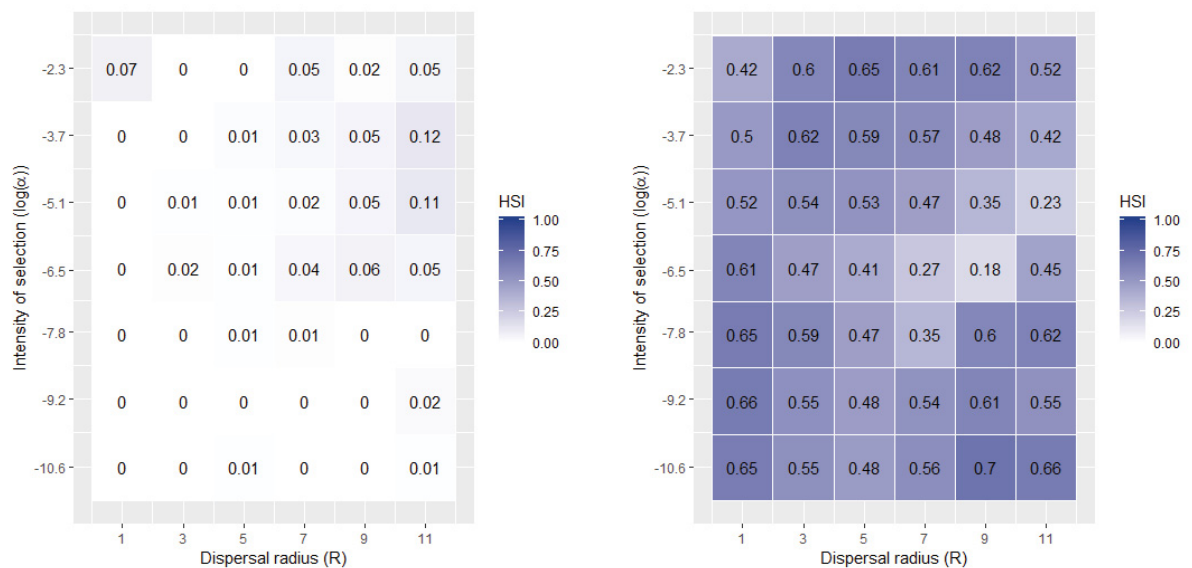


Figure S13. Host Specialization Index for the first speciation event for different values of dispersal radius (R) and intensity of selection (α). Left panel: measures for the lineage that retained most individuals at the speciation event; Right panel: measures for the lineages that retained fewer individuals at the speciation event.

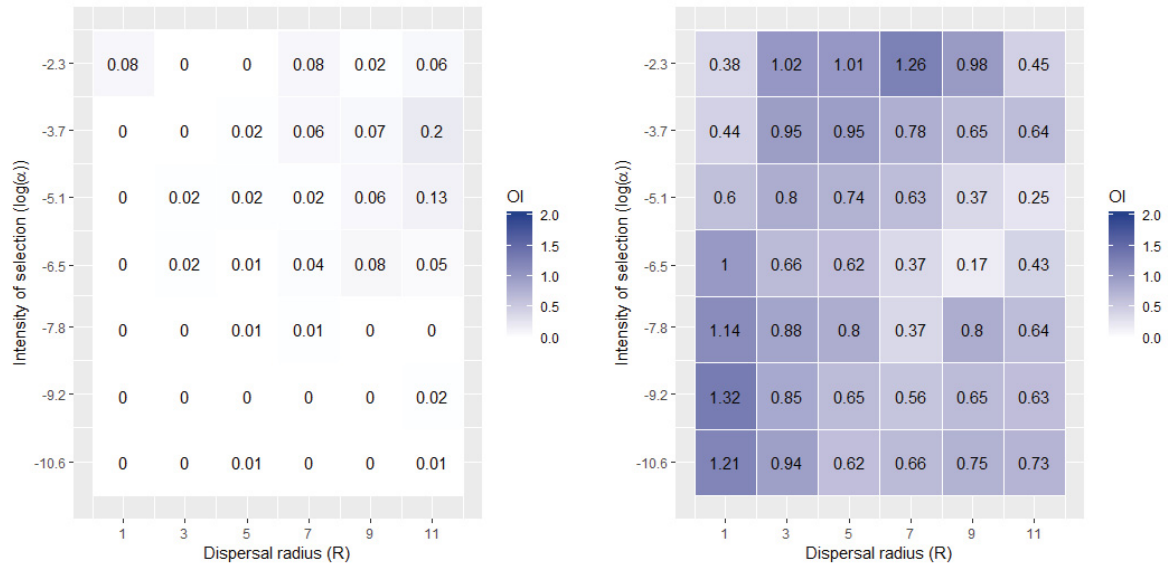


Figure S14. Oscillation Index for the first speciation event for different values of dispersal radius (R) and intensity of selection (α). Left panel: measures for the lineage that retained most individuals at the speciation event; Right panel: measures for the lineages that retained fewer individuals at the speciation event.

SUPPLEMENTARY MATERIAL 5

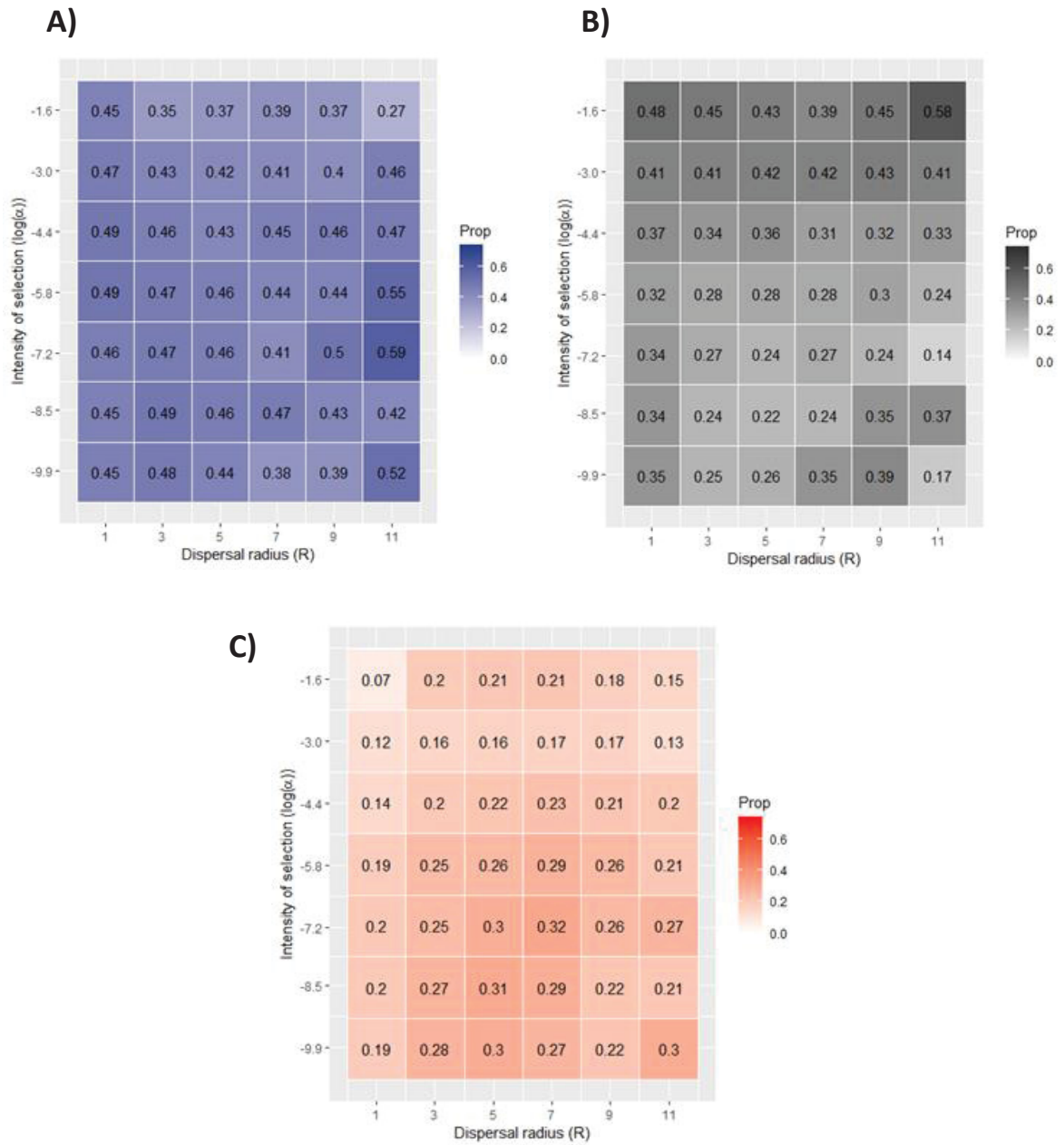


Figure S15. Proportion of events with Host Expansion Index values greater, equal or small than zero for different values of dispersal radius (R) and intensity of selection (α). The sign given by the HEI indicates the direction of variation on host range between a species origin and its next speciation event. A: Proportion of events with increase on host range (HEI > 0, proportion = 0.45 ± 0.05); B: Proportion of events with no variation on host range (HEI = 0, proportion = 0.33 ± 0.08); C: Proportion of events with decrease in host range (HEI < 0, proportion = 0.22 ± 0.05).

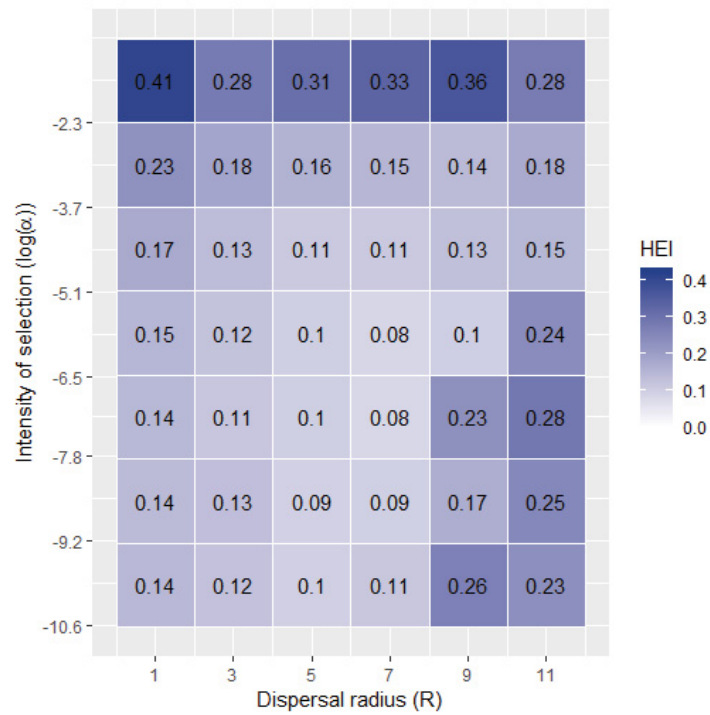


Figure S16: Mean Host Expansion Index for different values of dispersal radius (R) and intensity of selection (α).

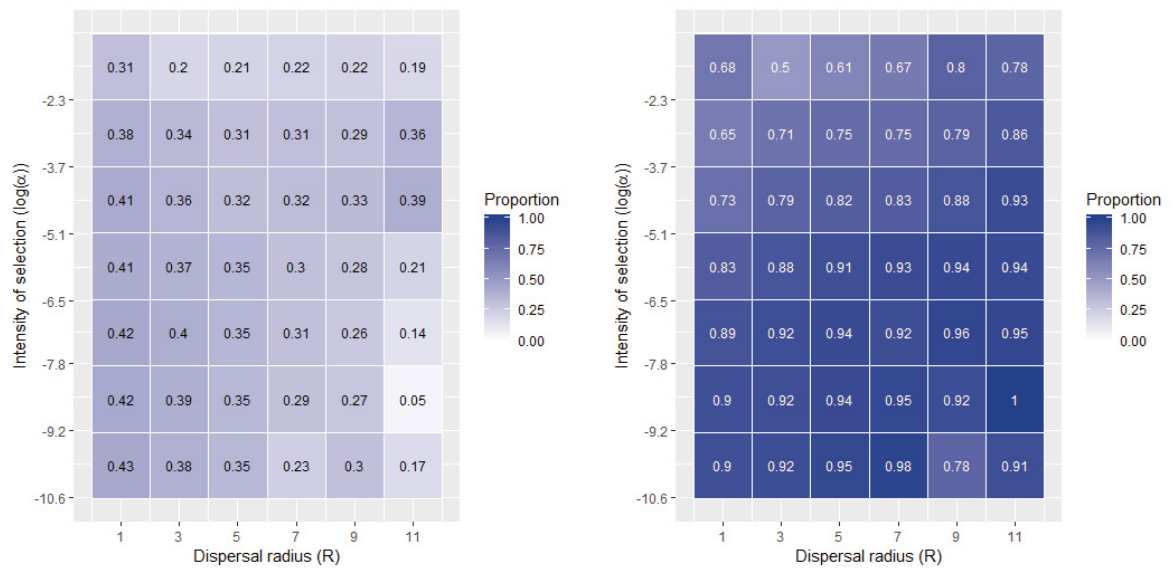


Figure S17. Proportion of events with specialization after the speciation events ($HSI > 0$) for different values of dispersal radius (R) and intensity of selection (α). Left panel: measures for the lineage that retained most individuals at the speciation event; Right panel: measures for the lineages that retained fewer individuals at the speciation event.

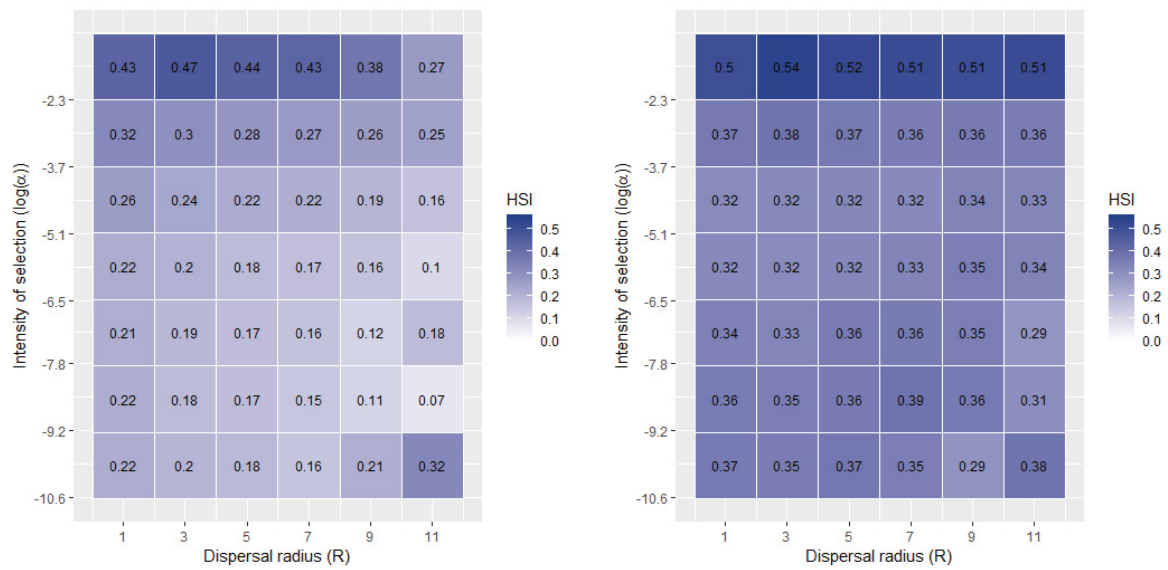


Figure S18. Mean Host Specialization Index when $HSI > 0$ for different values of dispersal radius (R) and intensity of selection (α). The values show the proportion of reduction on host range when it occurred after a speciation event. Left panel: measures for the lineage that retained most individuals at the speciation event; Right panel: measures for the lineages that retained fewer individuals at the speciation event.

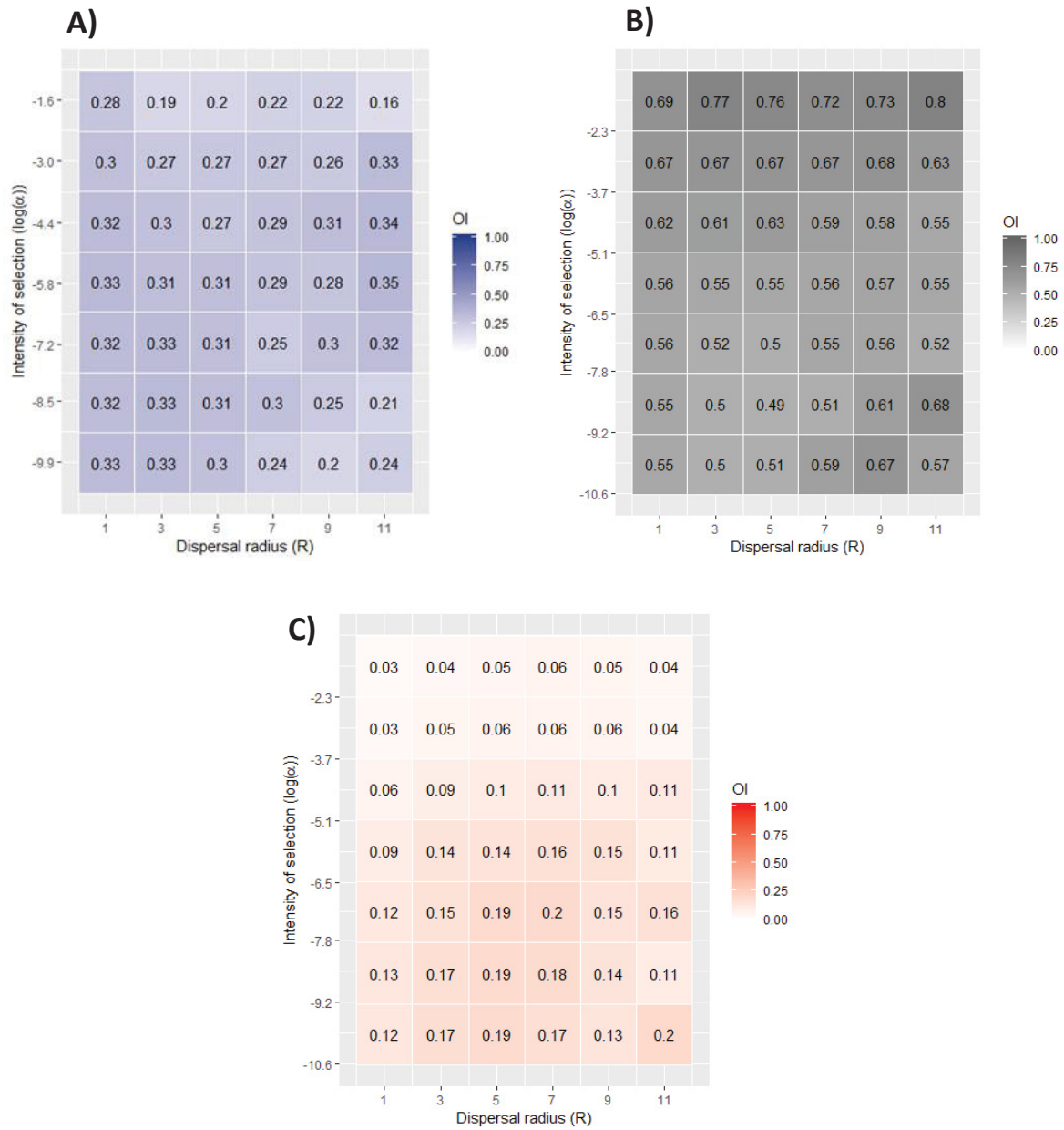


Figure S19. Proportion of events with Oscillation Index for different values of dispersal radius (R) and intensity of selection (α) when: A: the Oscillation Index is greater than zero; B: the Oscillation Index is equal to zero; C: the Oscillation Index is smaller than zero