

LETTER

Hybridization can promote adaptive radiation by means of transgressive segregation

Kotaro Kagawa^{1,2*} and
Gaku Takimoto³

Abstract

Understanding the mechanisms of rapid adaptive radiation has been a central problem of evolutionary ecology. Recently, there is a growing recognition that hybridization between different evolutionary lineages can facilitate adaptive radiation by creating novel phenotypes. Yet, theoretical plausibility of this hypothesis remains unclear because, for example, hybridization can negate pre-existing species richness. Here, we theoretically investigate whether and under what conditions hybridization promotes ecological speciation and adaptive radiation using an individual-based model to simulate genome evolution following hybridization between two allopatrically evolved lineages. The model demonstrated that transgressive segregation through hybridization can facilitate adaptive radiation, most powerfully when novel vacant ecological niches are highly dissimilar, phenotypic effect size of mutations is small and there is moderate genetic differentiation between parental lineages. These results provide a theoretical basis for the effect of hybridization facilitating adaptive radiation.

Keywords

Adaptive radiation, ecological speciation, evolutionary simulation, hybridization, individual-based model, sympatric speciation, transgressive segregation.

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INTRODUCTION

Understanding the mechanisms causing adaptive radiation is a fundamental challenge in evolutionary biology. In adaptive radiation, many ecologically diverse species rapidly evolve in a single taxonomic group (Schluter 2000). Since adaptive radiation by definition occurs in the face of ecological opportunities that foster adaptation into various vacant ecological niches (Schluter 2000), ecological speciation (*sensu* Nosil 2012) is considered a fundamental driver of adaptive radiation (Schluter 2000; Gavrillets & Losos 2009).

Recently, there is a growing recognition that hybridization between different evolutionary lineages can cause rapid diversification of ecological phenotypes and facilitate adaptive radiation (Seehausen 2004; Mallet 2009) (hereafter, hybrid adaptive radiation hypothesis). Indeed, genetic evidence of past hybridization events and their roles in phenotypic evolution has been reported in several major adaptive radiations (Seehausen 2004; Herder *et al.* 2006; Joyce *et al.* 2011; Abbott *et al.* 2013; Meier *et al.* 2017; Richards & Martin 2017). The mechanism underlying the hypothesis is the increase of genetic diversity through mixture of genes from different lineages. Hybrids' mosaic genomes aggregating genes from different parental lineages can create novel phenotypes. Such novel phenotypes, although mostly maladaptive, may occasionally facilitate adaptive invasion of hybrid organisms into novel ecological niches (Barton 2001; Mallet 2007). In addition,

hybridization and backcrossing can cause exchange of phenotypes among lineages by mediating gene introgression (Seehausen 2004; Jiggins *et al.* 2008), which has possibly facilitated the adaptive radiation of *Heliconius* butterflies (The *Heliconius* Genome Consortium 2012) and Darwin's finches (Lamichhaney *et al.* 2015).

Despite intuitive appeal, the hybrid adaptive radiation hypothesis has received little formal theoretical scrutiny. There are a number of theoretical uncertainties about the mechanisms and conditions by which hybridization may promote ecological speciation and adaptive radiation. First, the roles that transgressive segregation plays in hybrid adaptive radiation are poorly explored. Transgressive segregation, commonly found among hybrids (Rieseberg *et al.* 2003; Stelkens & Seehausen 2009), results from hybridization when multiple alleles with opposing phenotypic effects have fixed in parental lineages and recombination breaks down their compensating combinations (Rieseberg *et al.* 2003; Seehausen 2004). Transgressive segregation produces novel extreme phenotypes exceeding phenotypic range of parental lineages, and may facilitate adaptation and invasion by hybrids into novel niches. Although transgressive segregation is considered an important mechanism by which hybridization promotes ecological speciation (Gross & Rieseberg 2005; Mallet 2007; Rieseberg *et al.* 2007; Abbott *et al.* 2010, 2013; Dittrich-Reed & Fitzpatrick 2013), earlier theoretical models on hybrid speciation have not fully appreciated the roles of transgressive

¹The Institute of Statistical Mathematics, 10-3 Midori-cho, Tachikawa, Tokyo 190-8562, Japan

²Department of Fish Ecology and Evolution, Center for Ecology, Evolution & Biogeochemistry, Swiss Federal Institute of Aquatic Science and Technology, 6047 Kastanienbaum, Switzerland

³Graduate School of Agricultural and Life Sciences, The University of Tokyo, 1-1-1 Yayoi, Bunkyo-ku, Tokyo 113-8657, Japan

*Correspondence: E-mail: kagawakoutarou@gmail.com

segregation (McCarthy *et al.* 1995; Buerkle *et al.* 2000; Dueñez-Guzman *et al.* 2009; see discussion for more details). Moreover, although computer simulations have demonstrated that adaptive radiation can occur as a consequence of repeated ecological speciation (Gavrilets & Vose 2005; Ito & Dieckmann 2007; Aguilee *et al.* 2012; Birand *et al.* 2012), they did not consider the roles of hybridization, let alone the effects of transgressive segregation.

Second, there are several field examples that hybridization led to fusion of parental lineages into a single hybrid swarm (speciation reversal, Seehausen *et al.* 2008a; Vonlanthen *et al.* 2012), or population collapse by outbreeding depression or by the breakdown of local adaptation (Rhymer & Simberloff 1996; Todesco *et al.* 2016). Thus, hybridization may not only promote, but can also inhibit adaptive radiation. In particular, although preconditions for transgressive segregation require genetic differentiation between parental lineages (Stelkens & Seehausen 2009; Stelkens *et al.* 2009), hybridization between highly differentiated lineages could produce unviable/infertile offspring. Thus, conditions determining how hybridization promotes adaptive radiation might involve factors regulating the degree of genetic differentiation between parental lineages, such as the length of histories of their independent evolution, and the number and phenotypic effect size of genes underlying their phenotypic divergence.

Third, the conditions should be clarified under which a hybrid swarm with increased phenotypic variation can split into reproductively isolated species. A typical mechanism that causes reproductive isolation in ecological speciation is assortative mating based on ecological traits, which can automatically isolate ecologically differentiated populations (Coyne & Orr 2004; Nosil 2012). Such assortative mating commonly occurs in nature by habitat/temporal isolation between distinct ecotypes and/or by mate choice based on phenotypes (Coyne & Orr 2004; Servedio *et al.* 2011; Nosil 2012). However, previous theories have suggested that strong assortative mating can cause stabilising selection on ecological traits and inhibit ecological speciation (Kirkpatrick & Nuismer 2004; Otto *et al.* 2008). Thus, assortative mating can be an important ingredient of hybrid adaptive radiation by influencing the establishment of hybrid species.

Fourth, although solid evidence exists that past hybridization contributed to ecological diversification in some adaptive radiations (Meier *et al.* 2017; Richards & Martin 2017), it is wondered whether hybridization can be an essential cause of adaptive radiation (Richards & Martin 2017). Because large phenotypic variation caused through hybridization may allow hybrid organisms to cross fitness valleys and reach new adaptive peaks (Mallet 2007), hybridization may serve as an essential cause of adaptive radiation when radiation occurs on rugged fitness landscapes with fitness valleys. Ample evidence suggests that many adaptive radiations in real systems might have occurred on rugged fitness landscapes (Benkman 2003; Calsbeek & Irschick 2007; Hendry *et al.* 2009; Martin & Wainwright 2013; Arias *et al.* 2016). In contrast, former theoretical models on adaptive radiation have not explicitly addressed the difficulty of crossing fitness valleys when incipient species invade novel niches. Some models assumed that colonisers to novel empty niches could subsist without niche-

specific specialisation (e.g. Gavrilets & Vose 2005; Birand *et al.* 2012). Others assumed continuous niche axes, along which frequency-dependent competition caused gradual splitting of fitness peaks and allowed phenotypes to diverge without crossing fitness valleys (e.g. Dieckmann & Doebeli 1999; Ito & Dieckmann 2007; Aguilee *et al.* 2012). To examine whether hybridization is an essential cause of adaptive radiation, a theoretical model should test the roles of hybridization in adaptive radiation that involves the difficulty of crossing fitness valleys.

In this paper, we address the following four questions to theoretically examine the hybrid adaptive radiation hypothesis: (1) whether transgressive segregation through hybridization promotes adaptive radiation, (2) how genetic differentiation between parental lineages affects the likelihood of hybrid adaptive radiation, (3) what roles assortative mating plays in hybrid adaptive radiation and (4) whether hybridization can act as an essential cause of adaptive radiation. To answer these questions, we construct an individual-based model to simulate evolutionary dynamics following hybridization between two evolutionary lineages. To probe into detailed mechanisms underlying the conditions for hybrid adaptive radiation, we separately analyse two schemes differing in the number of novel ecological niches into which hybrid organisms can invade: (1) ecological hybrid speciation scheme – a simpler scheme in which there is a single novel ecological niche to be invaded by hybrid organisms, and (2) hybrid adaptive radiation scheme – a more complex scheme in which there are multiple novel ecological niches to be invaded by hybrids. We conduct simulations with and without hybridization to comparatively examine evolutionary effects of hybridization. Our simulation results demonstrate that hybridization can indeed promote adaptive radiation, and suggest specific conditions under which hybridization contributes to adaptive radiation.

MATERIAL AND METHODS

The model

General assumptions

The individual-based model simulates species multiplication at a secondary contact area of two parental lineages that have diverged in allopatry from a common ancestor (Fig. 1a). The model assumes three habitable sites (A, B and C), and N types of food resources (R_1, R_2, \dots and R_N). Sites A and B have only a single resource type (R_1), whereas site C has N types of resources including R_1 (i.e. R_1, R_2, \dots and R_N). In the ecological hybrid speciation scheme, $N = 2$; whereas in the hybrid adaptive radiation scheme, $N \geq 3$. At the start of simulation, 1000 individuals of the ancestral species are distributed randomly to sites A and B, and the respective populations spend T_1 generations separately without gene flow. Then, the two lineages of sites A and B (lineages A and B respectively) undergo a secondary contact at site C. Immigration from sites A and B into site C continues for T_2 generations at the migration rate m . After the immigration period, the simulation continues for another $T_3 - T_2$ generations (i.e. up to T_3 generations from the start of secondary contact). We test whether the

population in site C gives rise to new species that utilise novel resource types different from R_1 . This setting mimics a hypothesised scenario of adaptive radiation in real systems, in which temporal loss of geographic barrier or temporal expansion of distribution caused hybridization between genetically differentiated lineages, which facilitated early stages of adaptive radiation (e.g. Herder *et al.* 2006; Genner & Turner 2011; Hudson *et al.* 2011; Meier *et al.* 2017; Richards & Martin 2017). We did not consider evolution of intrinsic hybrid incompatibility (such as Bateson-Dobzhansky-Muller incompatibilities) because the time scale of our simulation is much shorter than the waiting time for development of complete post-zygotic isolation (typically, the order of millions of years; Coyne & Orr 2004).

Ecological feature of an individual i is characterised by a D -dimensional trait vector: $\mathbf{x}_i = (x_{i1}, \dots, x_{ij}, \dots, x_{iD})$, where x_{ij} is an evolving quantitative ecological trait and D is the number of traits. A trait vector \mathbf{x}_i determines the resource-use strategy of individual i . We assume an optimal trait vector $\mathbf{x}_{\text{opt}_r} = (x_{\text{opt}_r, 1}, \dots, x_{\text{opt}_r, j}, \dots, x_{\text{opt}_r, D})$ for a resource R_r . Individuals bearing the optimal trait vector $\mathbf{x}_{\text{opt}_r}$ can utilise the resource R_r with maximal efficiency (Fig. 1b). In addition to resource use, the trait vector affects the selection of mating partners; reproductive isolation can potentially develop

as a consequence of ecological differentiation in resource use. Each diploid individual has the genome consisting of $2n$ chromosomes of l base-pairs long (Fig. 1c). Each locus is of 5000 base-pairs long (Appendix S1) and locations of loci along the genome are assigned randomly before each simulation. Mutations on these loci affect trait values. A locus k of an individual i has one allele carrying a set of mutated nucleotides $M_{ik,1}$ and another allele carrying another set $M_{ik,2}$. New mutations are added to $M_{ik,1}$ and $M_{ik,2}$ upon meiosis at a constant rate μ per locus, and inherited over generations. A mutated nucleotide u in a locus alters locus' contribution to the trait value by a random amount ε_u , which follows a normal distribution $N(0, \sigma_m)$. Thus, the value x_{ij} of the j -th trait of an individual i is given as: $x_{\text{base}_j} + \sum_{k=1}^L \sum_{u \in \{M_{ik,1}, M_{ik,2}\}} \varepsilon_u$, where x_{base_j} is the common ancestral trait value. In addition to mutation, crossover recombination occurs on chromosomes at a rate of once per 10^8 base-pairs per generation (10^8 base-pairs correspond to a typical length of 100 centiMorgan in human genome; Lynch & Walsh 1998). The initial population is composed of clone individuals carrying two copies of the same haploid genome expressing a common trait vector, \mathbf{x}_{base} . More details on the simulation implementation of evolutionary processes are in Appendix S2.

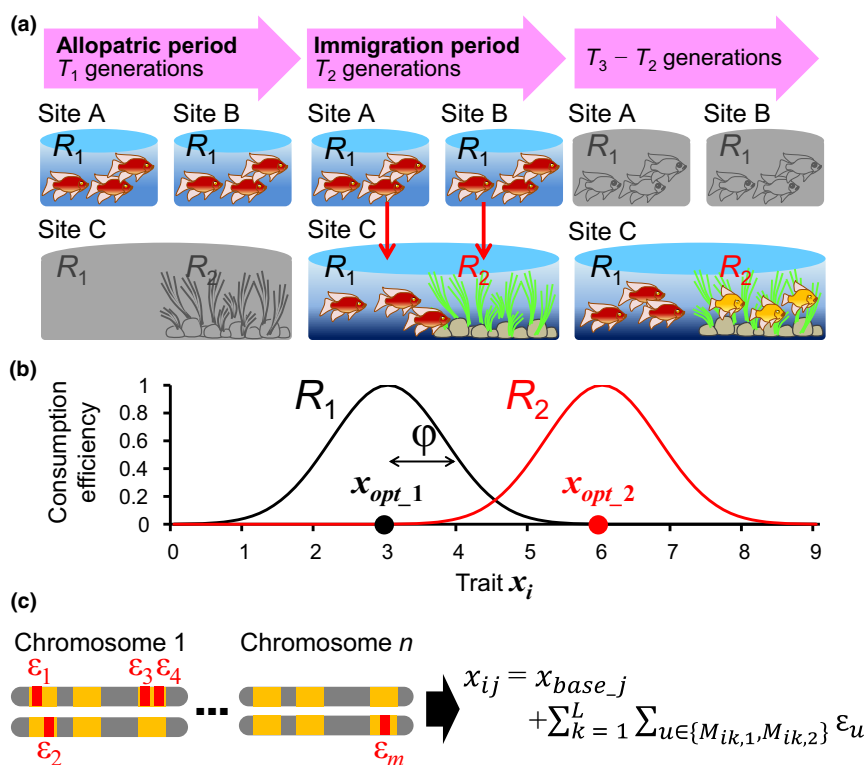


Figure 1 Overview of the model. (a) The simulation outline. The model considers three habitable sites A, B and C. At the start of simulation, the ancestral species establishes populations in sites A and B, and the respective populations spend T_1 generations separately without gene flow. Then, the two lineages of sites A and B undergo a secondary contact at site C. (b) Ecological trait of each individual i , \mathbf{x}_i , determines resource-use strategy of the individual. For each resource type r , there is an optimal trait set vector $\mathbf{x}_{\text{opt}_r}$ to effectively consume the resource. Parameter ϕ determines the level of specialisation in trait values required to utilise the resource. Thus, the value of ϕ determines the depth of fitness valleys between different adaptive peaks of a fitness landscape. (c) Genetic mechanism underlying phenotype determination. Genome of individuals consist of $2n$ chromosomes. A trait value x_{ij} is determined by the summed phenotypic effects of a set of L loci (shown as yellow squares). Only loci with changes from the ancestral sequence (shown as red squares) alter the trait value from the common ancestral trait value x_{base_j} (see main text for details).

Ecological interactions

We assumed non-overlapping generations to keep the model simple and lower computational load. Although non-overlapping generations may not be applicable to many adaptive radiations in real systems, qualitative results from the model should not be changed or this assumption might underestimate the likelihood of adaptive radiation (see Discussion). Two types of ecological interactions occur within a single generation: resource competition and mating. At every generation, a constant amount of resources is supplied to sites A, B and C (only R_1 is supplied to sites A and B, whereas all N types are supplied to site C). Individuals consume resources in their living site to survive to reproductive maturity. The amount of consumption C_{ir} of a resource R_r by an individual i is determined by three factors: the amount of resource supply (K_r), the maximum consumption rate of individual i (e_{ir}), and the summed maximum consumption rate of all individuals in the same site ($\sum_j e_{jr}$). C_{ir} is then given as:

$$C_{ir} = \begin{cases} e_{ir} & (K_r \geq \sum_j e_{jr}) \\ K_r e_{ir} / \sum_j e_{jr} & (K_r < \sum_j e_{jr}) \end{cases}$$

Resource competition occurs only when the summed maximum consumption rate exceeds the resource supply and reduces the amount of resource consumption from the maximum consumption rate e_{ir} . In such cases, C_{ir} is a fraction of the resource supply, which is proportional to the proportion of the individual maximum consumption rate in the summed maximum consumption rate of all individuals.

The maximum consumption rate e_{ir} of an individual i is determined by the matching between its trait vector x_i and the optimal trait vector x_{opt_r} for a resource R_r : $e_{ir} = \exp(-||x_{\text{opt}_r} - x_i||^2 / 2\varphi^2)$, where φ determines the degree of specialisation required to utilise the resource with smaller φ requiring greater specialisation. In other words, φ determines the depth of fitness valleys between different adaptive peaks of a fitness landscape. The probability that an individual i survives to maturation, S_i , increases with its total amount of resource consumption: $S_i = C_i / (\gamma + C_i)$, where $C_i = \sum_r C_{ir}$ is the total amount of resource consumption and γ is the resource consumption amount at which the survival probability is 0.5.

Surviving individuals form mating pairs for reproduction. When a mating pair is formed, a female is selected randomly from all females. Then, her mating partner is selected based on assortative mating that involves two processes: assortative mate encounter and assortative mate choice, which take place in this order. Assortative mate encounter can arise from habitat/temporal isolation between individuals using different niches, whereas assortative mate choice can arise from female preference toward mating partners.

In assortative mate encounter, a group of potential male partners are selected for each female on the basis of trait-value similarity between males and females. The probability of a male j being selected into the potential partner pool for a female i , $p_{e_{ij}}$, is: $p_{e_{ij}} = \exp(-\alpha_e^2 ||x_i - x_j||^2)$, where α_e is the strength of assortative mate encounter. The probability declines with ecological dissimilarity between males and females with larger α_e .

In assortative mate choice, a female chooses a single mating partner from candidate partners selected in assortative mate encounter. The probability that a male j is selected by a female i is given by $s_{ij} / \sum_j s_{ij}$, where s_{ij} indicates the rating of male j by female i based on their trait-value similarity. The rating s_{ij} is defined as: $s_{ij} = \exp(-\alpha_a^2 ||x_i - x_j||^2)$, where α_a measures the strength of assortative mate choice.

We assumed a monogamous mating system. Thus, individuals who have formed a mating pair are excluded from subsequent mating-pair formation. Mating-pair formation is repeated until any more pairs can be formed. Although mating-pair formation can be limited by several factors, such as resources, seasonality and timing for reproduction, our model did not incorporate them for simplicity. Each mating pair produces f offspring individuals that form the next generation.

Simulation settings

The ecological hybrid speciation scheme assumes only two types of resources in site C ($N = 2$), and only a single quantitative trait to evolve ($D = 1$). The optimal trait values for the two resources R_1 and R_2 are set to 3 and 6 respectively ($x_{\text{opt}_1} = 3$, $x_{\text{opt}_2} = 6$). The ancestral trait value x_{base} is set to x_{opt_1} .

The hybrid adaptive radiation scheme assumes 15 types of resources ($N = 15$) and three quantitative traits to evolve ($D = 3$). The optimal trait values for R_1 and the ancestral trait values are set to $x_{\text{opt}_1} = x_{\text{base}} = (3, 3, 3)$. The optimal trait values for the other 14 resource types are chosen as a set of three independent random variables following a uniform distribution $U(0, 6)$.

Parameter dependence analysis

To explore parameter conditions where hybridization facilitates and inhibits species multiplication, we performed simulations by systematically varying parameter values (Table 1). We focused on effects of the following parameters: mutational effect size σ_m , accessibility of resources φ , the length of allopatric period T_I , strengths of assortative mate encounter α_e and assortative mate choice, α_a . The empirical basis for our default parameter values and the detailed method of parameter dependence analysis are described in Appendices S1 and S3.

Simulations without hybridization

To explore how hybridization affects evolutionary dynamics, we conducted simulations without hybridization between lineages A and B. To suppress hybridization, we assumed that males of one lineage are not included into the pools of candidate mating partners of females of the other lineage; in other words, complete pre-mating reproductive isolation is considered to develop between the two lineages before their secondary contact.

Species count and categorisation of evolutionary outcomes

In both schemes of ecological hybrid speciation and hybrid adaptive radiation, we counted the number of ecologically distinct, reproductively isolated species. A single species is defined as a reproductively isolated cluster of individuals sharing similar trait values (Appendix S4). Evolutionary outcomes

Table 1 Model parameters

Definition	Symbol	Default values (ecological speciation)	Default values (adaptive radiation)	Values examined in parameter dependence analysis
The number of resources	N	2	15	—
The number of evolving traits	D	1	3	—
The number of chromosomes	n	15	15	5, 50
The length of each chromosome (bps)	l	2×10^8	2×10^8	6×10^7 , 6×10^8
The number of potential loci controlling a trait	L	5000	5000	1000, 2500, 5000, 10 000
Mutation rate/locus/generation	μ	0.5×10^{-5}	0.5×10^{-5}	—
Phenotypic effect size of a mutation	σ_m	$10^{-1.2}$	$10^{-1.6}$	10^{-2} , $10^{-1.8}$, $10^{-1.6}$, ... $10^{-0.4}$
The amount of resource supply	K	80	80	—
Female fecundity	f	10	10	—
The amount of resource consumption giving the survival probability 0.5	γ	1	1	—
Strength of assortative mate encounter	α_e	2^{-1}	2^{-1}	0 , 2^{-2} , $2^{-1.5}$, 2^{-1} , $2^{-0.5}$, ... 2^2
Strength of assortative mate choice	α_a	2^1	2^1	0 , 2^{-2} , $2^{-1.5}$, 2^{-1} , $2^{-0.5}$, ... 2^2
Accessibility of resources	φ	0.5	0.5	0.3, 0.4, 0.5, ... 0.8
The length of allopatric period	T_1	30 000	30 000	0, 5000, 10 000, 20 000, ... 15 000
The length of immigration period	T_2	1000	1000	5, ∞
The simulation duration after the start of secondary contact	T_3	2000	10 000	40 000
Migration rate in the immigration period	m	0.005	0.005	—

under the ecological hybrid speciation scheme were sorted into four categories based on the number of species in site C at the T_3 -th generation, their genetic composition, and their efficiency in utilising resources R_1 and R_2 . When site C contained more than two species and these species completely consumed R_1 and R_2 with no leftover, the dynamics were categorised as (1) ecological speciation. When site C had no individual, the dynamics were (2) population collapse. When the population in site C consisted only of genetically pure individuals of a single parental lineage, we categorised the result as (3) single lineage colonisation. When site C had only one species and individuals of this species carried alleles originating from both lineages A and B, the species was considered as a hybrid species; we categorised this outcome as (4) merge of parental lineages. If any of these categories were not applicable, outcomes were categorised as (5) others. This category included rare outcomes in which two ecologically distinct species occurred in site C without completely consuming the two resources.

RESULTS

Ecological hybrid speciation

Simulations of the ecological hybrid speciation scheme demonstrated both promoting and inhibiting effects of hybridization on speciation. We observed four categories of evolutionary outcomes: ecological speciation, population collapse, single lineage colonisation, and merge of parental lineages. In case of ecological speciation (Fig. 2a), transgressive segregation facilitated the formation of a new species. Before hybridization, trait-value distributions of parental lineages A and B were both maintained around $x = 3$, which is optimal for consuming the resource R_1 . Although the trait-value distribution changed only slightly during the allopatric period, different pairs of mutant genes whose complementary phenotypic effects cancel one another could have become

fixed in different populations (Fig. S2a). Such complementary genes, when their combinations are broken in hybrid/back-cross individuals, would produce novel phenotypic variants. Such novel phenotypes facilitated speciation, as shown in Fig. 2a. In this example, individuals of lineage A dominated site C right after the start of migration (the lower panel of Fig. 2a). Then, they hybridised with lineage B individuals and the site C population gradually accumulated genes from both lineages, which increased phenotypic variation. Although novel trait values of most hybrids were off the optimal values for consuming resources R_1 or R_2 , some hybrids with transgressive trait values established to form a new species that consumes resource R_2 efficiently and reproductively isolated from another species (the 752-th generation in Fig. 2a).

Evolutionary outcomes of population collapse (Fig. 2b) were observed typically when genetic differentiation between parental lineages was large. With much differentiation between parental lineages, hybridization produced overly large genotypic variation, and average trait dissimilarity between parents and their offspring increased as genetic admixture proceeded (Fig. S3). This made it difficult for hybrid individuals to maintain trait values suitable for consuming resources R_1 or R_2 . This eventually led to the extinction of the hybrid population. Single lineage colonisation (Fig. 2c) was observed when hybridization caused population collapse and then only one lineage re-colonised afterwards. Merge of parental lineages (Fig. 2d) occurred, in which two parental lineages fused into a single hybrid swarm. This was observed when genetic differentiation between parental lineages was small, or when assortative mating was weak.

Hybridization significantly elevated the possibility of ecological speciation especially when the novel niche is separated from the original niche by a large fitness valley. We compared simulations with and without hybridization across the gradient of resource accessibility φ and mutational effect size σ_m (Figs 3a, S4). With hybridization, speciation was dominant outcomes except when φ was very small. On the other hand,

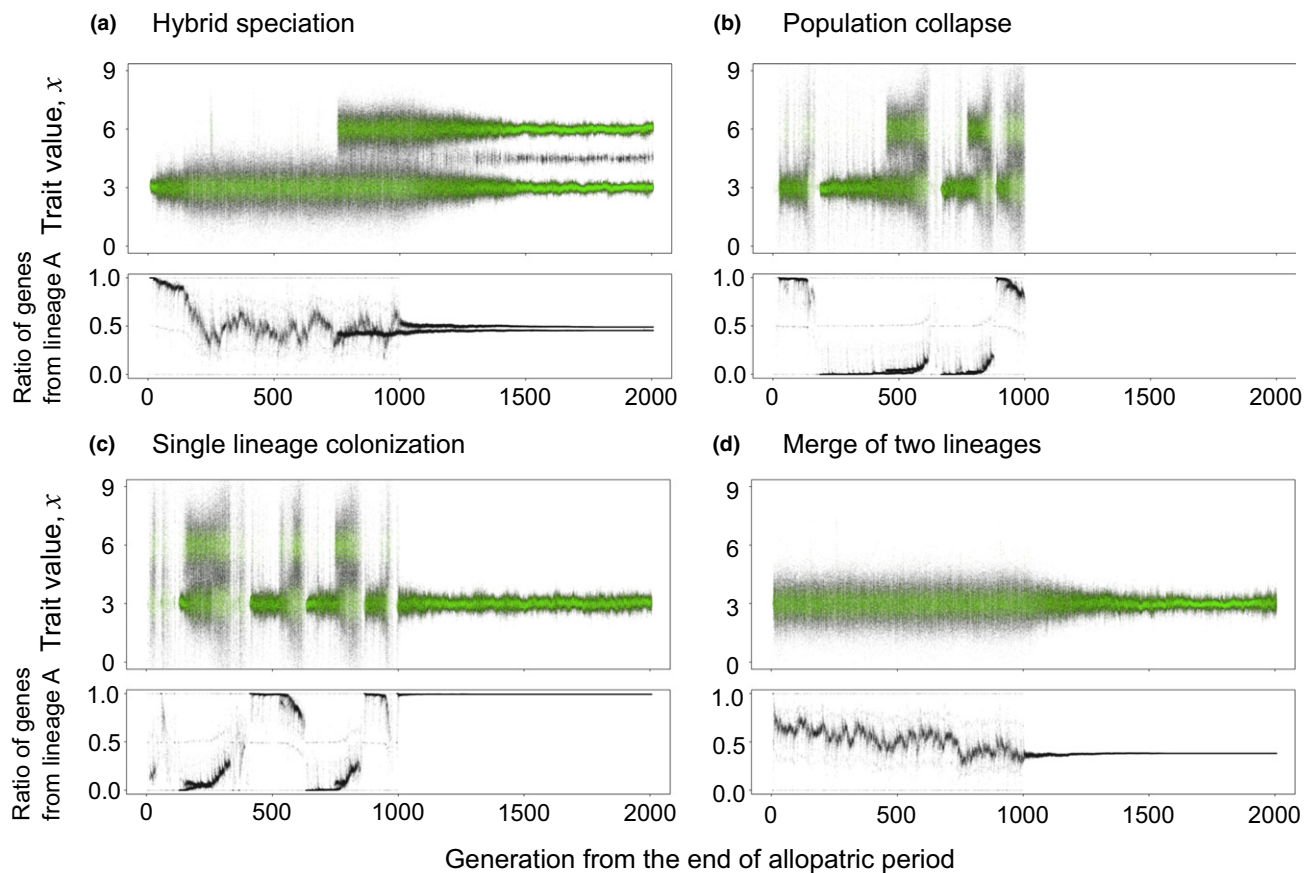


Figure 2 Examples of evolutionary dynamics following hybridization in the ecological hybrid speciation scheme. Upper panels: dynamics of trait value x . Trait values of all individuals in site C are shown in each generation. Individuals who survived to maturation and died before maturation are shown in green and grey respectively. Lower panels: genetic composition of all individuals. The vertical axis shows the ratio of genes from the lineage A in genomes of individuals (individuals with the ratio 1 and 0 are pure lineage A and B, whereas individuals with intermediate ratios have hybridised genomes). (a) Ecological speciation ($L = 5000$, $\sigma_m = 10^{-1}$, $\phi = 0.4$). (b) Population collapse ($L = 10\,000$, $\sigma_m = 10^{-1}$, $T_1 = 100\,000$). (c) Single lineage colonisation ($L = 10\,000$; $\sigma_m = 10^{-1}$; $T_1 = 70\,000$). (d) Merge of parental lineages ($L = 10\,000$, $\sigma_m = 10^{-1}$, $\alpha_e = 2^2$, $\alpha_a = 0$). Other parameters were set to the default values (Table 1).

without hybridization, speciation was possible only when both resource accessibility and mutational effect size were high. Instead, single lineage colonisation (Fig. S1) resulting from competitive exclusion was dominant outcomes, since parental lineages could not merge under prohibited hybridization. Additional simulations for much longer generations ($T_3 = 40\,000$) confirmed that low likelihood of speciation in the absence of hybridization was not due to short simulation duration (Fig. S5). The finding that hybridization facilitated ecological speciation was robust over a wide range of model assumptions. The same pattern was found (1) with a model relaxing the assumption that assortative mating is based on ecological traits (Fig. S6), (2) with short and long immigration period (Fig. S7), (3) with large and small numbers of chromosomes (Fig. S8) and (4) when parental lineages were assumed to adapt different ecological niches (Figs S9, S10).

In simulations with hybridization, the degree of genetic differentiation between parental lineages strongly affected evolutionary outcomes. Multiple factors, including the length of period for allopatric evolution of parental lineages (T_1), the mutational effect size (σ_m) and the number of potential loci controlling the trait x (L), affected the degree of genetic

differentiation, which was measured by an index GD (Appendix S5). Variation in GD correlated closely with relative likelihood of different evolutionary outcomes (Figs 4a, S11). When T_1 was small, GD was low and hybridization mostly resulted in merge of parental lineages. When T_1 was not small, GD was intermediate and speciation was dominant outcomes. When T_1 was large and σ_m was intermediate, large GD was attained, and population collapse and colonisation of a single lineage were major outcomes (Fig. 4a). When σ_m was larger, GD was rather decreased probably because stabilising selection in sites A and B immediately excluded mutant genes having large phenotypic effects. Large L accelerated the increase of GD at intermediate σ_m and large T_1 (Fig. S11).

Either assortative mate encounter or assortative mate choice needed to be strong enough for reproductive isolation to develop and speciation to occur (Fig. 5a). However, too strong assortative mate encounter (too large α_e) inhibited speciation (Figs 5a, S12, S13). This is probably because strong assortative mate encounter reduced the chances that individuals invading novel niches successfully found their mating partners (see Discussion for more details).

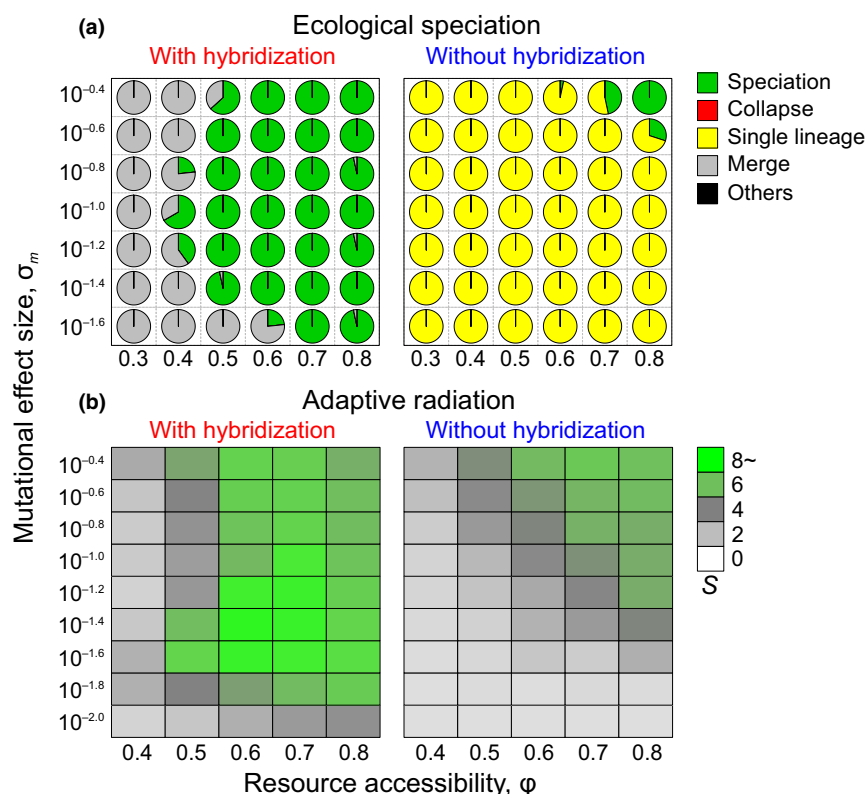


Figure 3 Effects of hybridization, mutational effect size σ_m , and resource accessibility ϕ . (a) Results in the ecological hybrid speciation scheme. Left: with hybridization. Right: without hybridization. Each pie chart shows frequencies of five categories of evolutionary outcomes in 30 simulation runs. (b) The hybrid adaptive radiation scheme. Left: with hybridization. Right: without hybridization. Depth of green colour shows the average number of species S at the end of simulation across 30 runs. Other parameters: default values in the Table 1

Hybrid adaptive radiation

Simulations of the hybrid adaptive radiation scheme demonstrated that hybridization could promote adaptive radiation. In an example case (Fig. S14), nine reproductively isolated species evolved to use different resources within 10 000 generations.

Parameter dependence analysis found that overall effects of parameters were qualitatively similar to those under the ecological hybrid speciation scheme. Hybridization promoted adaptive radiation across broad ranges of resource accessibility ϕ and mutational effect size σ_m (Figs 3b, S15). Regardless of whether hybridization was permitted, large ϕ tended to decrease the resultant number of species because high resource accessibility favoured evolution of a few generalist species rather than many specialists. Hybrid adaptive radiation was most likely with values of the allopatric period length (T_1) and mutational effect size (σ_m) that produced moderate genetic differentiation between parental lineages before hybridization (Figs 4b, S16). By contrast, parameter combinations that produced large genetic differentiation between parental lineages hindered adaptive radiation, probably because too large phenotypic variation in hybrid populations hindered their adaptation to novel niches. Stronger assortative mate choice (larger α_a) promoted adaptive radiation, whereas stronger assortative mate encounter (larger α_e) failed to promote adaptive radiation (Figs 5b, S17).

DISCUSSION

The hybrid adaptive radiation hypothesis predicts that hybridization between different evolutionary lineages can cause rapid phenotypic diversification and facilitate adaptive radiation (Seehausen 2004). However, the mechanisms and conditions underlying the hypothesis have remained theoretically unexplored. To investigate detailed mechanisms of how hybridization promotes ecological speciation and adaptive radiation, we developed and analysed an individual-based evolutionary simulation model in which two parental lineages independently evolve in separation and then secondarily contact to hybridise. We discuss the obtained results in terms of the four potentially important factors raised in the questions in the introduction.

Transgressive segregation

There are three pioneering simulation models that have studied hybrid speciation (McCarthy *et al.* 1995; Buerkle *et al.* 2000; Duenez-Guzman *et al.* 2009). These models analysed the likelihood of recombinational speciation under a variety of genetic and ecological contexts. The model by McCarthy *et al.* (1995) considered hybridization between two species differing by two or more chromosomal rearrangements that cause partial sterility of heterozygotes. Their simulation has shown that hybridization can form a new species of a novel

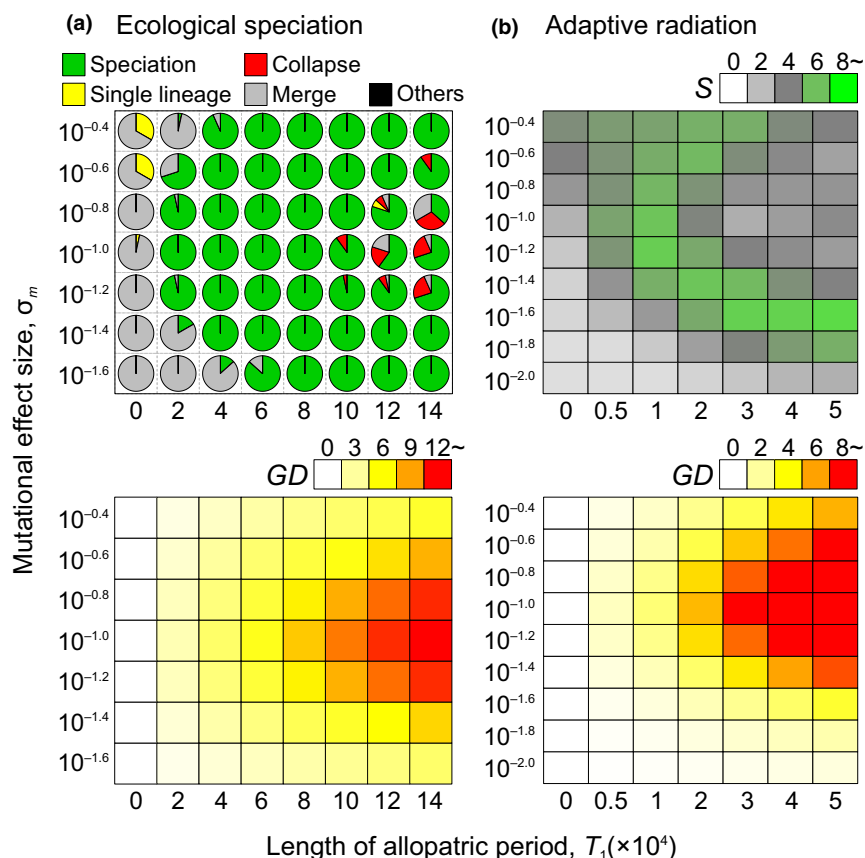


Figure 4 Effects of the mutational effect size σ_m , and the length of allopatric period T_1 . (a) The ecological hybrid speciation scheme. Upper: frequencies of five categories of evolutionary outcomes. Lower: the degree of genetic differentiation between parental lineages at the end of allopatric period (averaged across 30 runs) (GD). (b) The hybrid adaptive radiation scheme. Upper: the average number of species S at the end of simulation. Lower: the degree of genetic differentiation (GD). Other parameters: default values in the Table 1

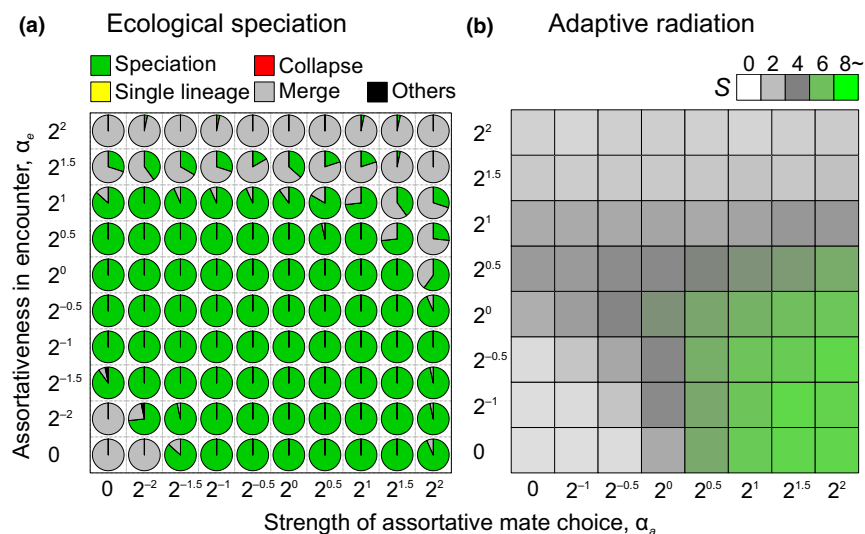


Figure 5 Effects of strengths of assortative mate encounter α_e and assortative mate choice α_a . (a) The ecological hybrid speciation scheme. Pie charts show frequencies of five categories of evolutionary outcomes. (b) The hybrid adaptive radiation scheme. Depth of green colour shows the average number of species S at the end of simulation. Other parameters were set to the default values (Table 1).

recombinant homozygous genotype, which is fully fertile and reproductively isolated from parental species by chromosomal sterility barrier. The model by Buerkle *et al.* (2000) considered an ecological trait subject to habitat-specific selection in addition to incompatible chromosomal inversions causing partial heterozygote sterility, and showed that a hybrid species could be established in a novel habitat unfavourable for parental species. The genetics determining the ecological trait, although mimicking those causing transgressive segregation (Buerkle *et al.* 2000), does not consider the possibility that transgressive segregation can produce various phenotypes no more favoured than parental phenotypes in the novel habitat. Finally, Duenez-Guzman *et al.* (2009) tailored a model specific to a probable case of ecological hybrid speciation of *Heliconius* butterflies. Their model demonstrated that a recombinant hybrid species bearing wing coloration of both parental species could be established.

Our model complements these previous models by exploring the effects of hybridization causing transgressive segregation on ecological speciation and adaptive radiation. In our model, transgressive segregation through hybridization, unlike mutation accumulation, enabled instantaneous and repeated formation of potentially adaptive novel phenotypes through assembling genetic materials from parental lineages into novel genotypes, thereby promoting ecological speciation and adaptive radiation. This result lends theoretical support for the hypothesised contribution of transgressive segregation in some empirical cases of ecological hybrid speciation (Rieseberg *et al.* 2007; Abbott *et al.* 2010; Ditttrich-Reed & Fitzpatrick 2013).

Genetic differentiation between parental lineages

Phenotypic variation created through transgressive segregation did not only promote, but could also inhibit adaptive radiation by causing the collapse of hybrid populations. Too large phenotypic variation decreased the mean fitness of hybrids to such low levels that hybrid populations became unsustainable and collapsed. Such large phenotypic variation was produced when there was much differentiation between hybridising lineages. This finding may correspond to empirical observation that hybridization between genetically distant lineages increased the risk of extrinsic or intrinsic outbreeding depression (Coyne & Orr 2004; Toderico *et al.* 2016). We thus predict that the likelihood of hybrid adaptive radiation might be highest when genetic differentiation between parental lineages is moderate.

Our model considered that parental lineages had separately adapted to the same ecological niches. Yet, different modes of parental lineage evolution could affect their genetic differentiation and consequences of their hybridization. For example, unlike our assumption, parental lineages could have adapted to different niches. Our preliminary analysis relaxing this assumption found that transgressive hybrids of differentially adapted parental lineages could facilitate ecological speciation (Fig. S10), although more extensive analysis should be necessary for a robust conclusion. Moreover, different types of evolutionary forces (e.g. stabilising, directional, or divergent natural selection, or genetic drift) can accumulate different

sorts of genetic differentiation between parental lineages and affect the likelihood of transgressive segregation (Albertson & Kocher 2005). Detailed analysis on this regard would elaborate the conditions for hybrid adaptive radiation through transgressive segregation.

Assortative mating

Previous theories have suggested that too strong assortative mating on ecological traits can, by keeping novel rare types from acquiring mating partners, cause stabilising sexual selection and inhibit speciation (Kirkpatrick & Nuismer 2004; Otto *et al.* 2008). In accord with this view, our results found that while adaptive radiation requires assortative mating, too strong assortative mate encounter inhibited speciation. In contrast, strong assortative mate choice did not inhibit speciation. This was probably because mate choice did not cause difference in mating success among individuals under the monogamous system of our model. Although not incorporated in our model, intermittent asexual reproduction or overlapping generations may mitigate the inhibitory effect of stabilising sexual selection. Generation overlaps would allow for longer waiting time until organisms of rare phenotypes find similar mating partners.

Hybridization as an essential cause of adaptive radiation

Empirical evidence that hybridization contributed to several adaptive radiations provoked the question whether hybridization could be an essential cause of adaptive radiation (Richards & Martin 2017). Our model demonstrated that the effect of hybridization to promote adaptive radiation was most pronounced when novel niches were separated by large fitness valleys, because transgressive phenotypes can jump fitness valleys to reach distant adaptive peaks. On this basis, we suggest that hybridization causing transgressive segregation can be an essential cause of adaptive radiation that occurs on highly rugged fitness landscapes.

CONCLUSIONS

Our theoretical analysis supports the hybrid adaptive radiation hypothesis. Our results predict that hybridization may promote adaptive radiation most powerfully when there is moderate genetic differentiation between parental hybridising lineages, and when large fitness valleys separate highly dissimilar novel niches. In addition, our simulation found that transgressive segregation can explain the origin of high evolvability in lineages undergoing adaptive radiation – a point that few formal models of adaptive radiation have explicitly considered. These theoretical predictions should be tested in real case examples of adaptive radiation.

We note that our model did not incorporate several important and intriguing aspects of adaptive radiation in real systems. For example, adaptive radiation can itself create novel ecological niches. Newly emerging species could themselves serve as novel trophic resources, which might facilitate further evolution of predatory species from the same clade (Ingram *et al.* 2009; Losos 2010). Joint action of natural and sexual

selection can be another powerful driving force of adaptive radiation, as suggested from a candidate example of hybrid adaptive radiation in cichlids involving multiple sensory-drive speciation (Seehausen *et al.* 2008b; Meier *et al.* 2017). An important future challenge may be to explore the effects of phenotypic variance created by hybridization in such dynamic and multitiered adaptive radiation.

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AUTHOR CONTRIBUTIONS

KK and GT designed the study; KK developed the computer simulation model and conducted analyses; KK wrote the manuscript together with GT.

DATA ACCESSIBILITY STATEMENT

Java source codes of our individual-based simulation models, R scripts that we used to produce figures, and simulation results in this paper are available from the Dryad Digital Repository (<https://doi.org/10.5061/dryad.4cf2p>).

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SUPPORTING INFORMATION

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