DISRUPTIVE SELECTION AS A DRIVER OF EVOLUTIONARY BRANCHING AND CASTE EVOLUTION IN SOCIAL INSECTS

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Abstract. Theory suggests that evolutionary branching via disruptive selection may drive substantial phenotypic divergence as part of the speciation process. Here, we extend this theory to social insects, which have novel social axes of phenotypic diversification. Our model, built around turtle ant (*Cephalotes*) biology, is used to explore whether disruptive selection can drive the evolutionary branching of divergent colony phenotypes that include a novel soldier caste. Soldier evolution is a recurrent theme in social insect diversification exemplified in the turtle ants. We show that phenotypic mutants can gain competitive advantages that induce disruptive selection and subsequent branching. A soldier caste does not generally appear before branching, but can evolve from subsequent competition. The soldier caste then evolves in association with specialized resource preferences that maximize defensive performance. Overall, our model indicates that resource specialization may occur in the absence of morphological specialization, but that when morphological specialization evolves, it is always in association with resource specialization. This evolutionary coupling of ecological and morphological specialization is consistent with recent empirical evidence, but contrary to predictions of classical caste theory. Our model provides a new theoretical understanding of the ecology of caste evolution that explicitly considers the process of evolution.

1. INTRODUCTION

How ecology shapes phenotypic diversification remains a central question in the field of evolutionary biology. There has been a resurgence of interest in this question in recent years, including a significant amount of new theoretical and empirical work on "ecological speciation" (reviewed in Schluter, 2000; Rundle and Nosil, 2005; Rueffler et al., 2006; Weissing et al., 2011; Nosil, 2012; Rabosky, 2013). Broadly defined, ecological speciation is the production of new species from ecologically-based divergent selection between environments (derived from Schluter, 2000; Nosil, 2012). This general process may result from a number of specific ecological scenarios, but most are expected to produce phenotypically divergent daughter species, each adapted to the environment it inhabits (Nosil, 2012). This mode of speciation is therefore thought to be key in driving adaptive phenotypic diversification within lineages, but much is still to be learned about the different stages of this process, the conditions that favor it, and its prevalence across taxa (Nosil, 2012).

Among the different ecological scenarios that favor ecological speciation, competition within a population, resulting in disruptive selection, may be particularly powerful in driving phenotypic divergence (Nosil, 2012). Disruptive selection can be seen as a special form of divergent selection where a more common phenotype in the population has a fitness disadvantage with respect to low-frequency phenotypic extremes (e.g., Bolnick, 2004; Bolnick and Lau, 2008; Calsbeek and Smith, 2008; Martin and Pfennig, 2009; Hendry et al., 2009). By gaining access to resources that are being competed over less intensely, individuals with the extreme phenotypes have higher fitness, driving up the tails of the phenotypic distribution, without associated changes in the underlying resource distribution. If this phenotypic and ecological divergence also results in a significant degree of reproductive isolation among the phenotypic extremes, either directly or indirectly, speciation may follow (Rueffler et al., 2006; Weissing et al., 2011; Nosil, 2012). The result is two daughter species with adaptive phenotypic differences that are maximally divergent within the bounds of the original phenotypic distribution. This process, although previously seen as controversial or at least rare, is now thought to be relatively common when appropriate ecological conditions prevail (Rueffler et al., 2006; Nosil, 2012). Nevertheless, recent advances in the theoretical and empirical understanding of ecological speciation via disruptive selection have been relatively limited in taxonomic representation, entirely within the realm of "unitary" organisms (see reviewed case studies in Nosil (2012)). It is therefore likely that much is still to be learned from work on underrepresented taxa, especially those that typically interact in ecological contexts favorable to disruptive selection.

Derived social insect taxa have been entirely overlooked with respect to work on disruptive selection and ecological speciation. These taxa have undergone a transition in biological complexity (Bourke, 2011) such that the colony operates as an integrated adaptive unit (Strassman and Queller, 2010; Pepper and Herron, 2008). This gap is significant for a number of reasons. The first is simply the evolutionary and ecological significance of this group. For instance, the ants alone have diversified to over 13,000 described species, undergone repeated bursts of adaptive radiation, and today represent a diverse and ecologically dominant fauna worldwide, especially in the tropics (reviewed in Lach et al. (2010)). Second, little work has been done on mechanisms of speciation in social insects, and existing theory to explain phenotypic diversification (Oster and Wilson, 1978) does not explicitly account for the evolutionary process. Third, although this same theory has inspired a considerable amount of social insect research, it is now over 35 years old and there has been weak to no support for many of its central premises and predictions for phenotypic diversification (e.g. (Walker and Stamps, 1986; Kaspari and Byrne, 1995; Ferster et al., 2006; Powell, 2009)). Finally, social insects have numerous axes of phenotypic diversification not seen in unitary organisms. For instance, selection has favored the evolution of phenotypically and functionally differentiated individuals or, "castes", within the colonies of many species. Individuals of different castes then serve as different traits of the functionally integrated organismal colony (Powell, 2008; Strassman and Queller, 2010). Furthermore, overall colony structure, including the presence and absence of certain castes and their relative representation, adds additional axes. We would argue that these complex social axes of phenotypic diversification have previously served to isolate social insect research from mainstream evolutionary theory. Nevertheless, this isolation may have obscured commonalities in processes and patterns of phenotypic diversification across levels of biological complexity.

Here we extend the theoretical framework for evolutionary branching via disruptive selection to social insects. We focus on the capacity for resource competition and disruptive selection to drive the evolution of daughter phenotypes with novel defense traits, represented by a "soldier" caste. Soldier evolution is one of the major, recurrent themes in the diversification of social insects, with independent origins in 6 major insect lineages (ants: Dornhaus and Powell, 2010; aphids: Stern, 1994; polyembryonic wasps: Cruz, 1981; stingless bees: Grüter et al., 2012; termites: Thorne et al., 2003; thrips: McLeish and Chapman, 2007). In addition, soldiers have evolved multiple times independently in the ants, including in some of the most diverse and ecologically important genera (Baroni Urbani, 1998; Dornhaus and Powell, 2010). The classical caste evolution theory predicts that specialized castes like soldiers should evolve when the species expands the breadth of resources the colony uses (Oster and Wilson, 1978). However, recent empirical work with the charismatic turtle ants (*Cephalotes*) suggests the opposite: the evolution of a specialized soldier caste is associated with species using more specialized nesting resources (Powell, 2008, 2009). Turtle ants have armored heads used to defend the entrances of the pre-existing arboreal cavities that they find in the environment and inhabit (Figure 1; (Creighton and Gregg, 1954; Powell, 2008, 2009)). The use of an increasingly narrow range of entrance sizes is then associated with a number of discrete transitions in the evolution of a specialized soldier phenotype, with the first transition being the one from no soldier to soldier present (Powell, 2008). These significant phenotypic shifts in association with species using a narrower set of resources is broadly consistent with the pattern expected under ecological speciation via disruptive selection (Rueffler et al., 2006; Nosil, 2012), and inconsistent with existing caste evolution theory (Oster and Wilson, 1978).

Critically, other aspects of turtle ant biology are consistent with the broad ecological scenario thought to favor ecological speciation via disruptive selection. First, the arboreal, pre-existing cavities used as nests by turtle ants are also used by most other arboreal ant taxa (Powell et al., 2011), are a limited resource in diverse tropical systems (Philpott and Foster, 2005; Powell et al., 2011), and aggressive cavity usurpation is common (Powell, 2009). This highly competitive environment is likely to favor the negative frequency dependent fitness dynamics that underlies the process of disruptive selection. Second, a mismatch between ant head dimensions and the size of the cavity entrance-hole can significantly increase the likelihood of cavity usurpation and mortality in turtle ants (Powell, 2009). These strong fitness consequences associated with the specificity of the phenotype-resource association are likely to amplify the advantages of rare phenotypic extremes within the population. Finally, the phenotype of extant sister species tends to be most differentiated with respect to soldier morphology (De Andrade and Baroni Urbani, 1999), and members of sister pairs are often sympatric in diverse contemporary turtle ant assemblages (De Andrade and Baroni Urbani, 1999). These patterns are consistent with an evolutionary history of ecological speciation via disruptive selection, with the ecological relationship between cavity hole and head morphology being the driver.

In this paper, we use this rich knowledge of turtle ant biology to develop a model for phenotypic divergence via disruptive selection based on the Adaptive Dynamics framework (AD; Metz et al. (1996); Geritz et al. (1997, 1998); Dercole and Rinaldi (2008)). Using a structured metapopulation model to describe occupancy of nests with different entrance sizes blocked by soldier ants, we incorporate the mechanisms by which worker size distribution influences nest preferences and defensive abilities. We then investigate if the evolutionary dynamics of worker size distributions converge to evolutionary branching points, and if at such points phenotypic divergence causes castes to form.

2. METHODS

2.1. **Modelling *Cephalotes*.** The Adaptive Dynamics model has two components: one containing ecological dynamics, and one with evolutionary dynamics. See Figures 2 and 3 for illustrations of the main concepts. On the ecological timescale, colonies with different traits compete over nest resources, with either an eventual winner (all colonies having the same phenotype) or coexisting set of colonies as a result. Then in each evolutionary time step, a small fraction of the resident colonies mutates to have slightly different traits. The ecological competition dynamics are then played out again, with new long-term residents as a result. In this way, the traits of resident colonies slowly changes on the evolutionary time scale, giving rise to evolutionary dynamics, and potentially evolutionary branching.

At this level, our use of Adaptive Dynamics is straightforward. Our model contains several noteworthy ingredients, however. First, since the nest size distribution is not set by the ants (but by wood-boring beetles), the ecological dynamics are assumed to take the form of metapopulation dynamics. Second, the ecological dynamics are infinite-dimensional, creating some mathematical challenges. Third, to distinguish between unimodal and bimodal ant worker size distributions, we model such distributions with three traits. (Most AD models describe the evolution of only one trait.)

2.2. **Ecological model.** From the wide array of possible model descriptions available (Bolker, 2004; Ovaskainen and Hanski, 2004), we focus on the simplest and classical description of metapopulation dynamics, the Levins model (Levins, 1970). We start with equations for two phenotypes within a population competing over some resource. These are given by

$$\frac{dy}{dt} = c_y y(1-y-z) - e_y y, \tag{1}$$

$$\frac{dz}{dt} = c_z z(1-y-z) - e_z z. \tag{2}$$

Here y and z denote the fraction of patches occupied by phenotype 1 and 2 respectively, c_y and c_z are the respective colonization rates and e_y and e_z the extinction rates. The term $1-y-z$ is thus the fraction of empty patches. See Nee and May (1992, 1997) and May and McLean (2007) for details of such competition models.

To include the relevant biology for *Cephalotes*, we introduce several extra ingredients. We assume there is a fixed distribution of resources $h(x)$, which we interpret as the distribution of nest cavities with given entrance width x (illustrated in Figure S1 in the Supplementary Information (SI)). Let $y(x,t)$ denote the number of nest cavities with width x occupied by colonies of phenotype 1 at time t, and similarly $z(x,t)$ for phenotype

2. Let $\int h(x)\,dx = 1$ be the total number of patches, normalized to 1, and let Y and Z denote the total fraction of patches occupied by phenotype 1 and 2 resp., so

$$Y(t) = \int y(x,t)\,dx, \quad Z(t) = \int z(x,t)\,dx.$$

(We typically suppress the integral boundaries, but $[0, L]$ for L large but finite suffices everywhere in this paper.) Colonies vacate a patch due to a natural death rate e which for simplicity is assumed neither to depend on the phenotype, nor on the phenotype's colony size distribution.

Second, phenotypes are assumed to have a preference profile $g_y(x)$ or $g_z(x)$, which determines the relative preference for patches of different width x. No preference for phenotype 1 would mean $g_y(x)$ is identically equal to some constant. To incorporate the preference function in the equations, we need to weight it with the distribution of nest resources $h(x)$. To this end, we set

$$H_y := \int g_y(x)h(x)\,dx.$$

If $g_y \equiv 1$, then of course, $H_y = 1$.

Including these two extensions gives a basic metapopulation model for resource distributions,

$$\frac{dy}{dt}(x,t) = c_y \frac{g_y(x)}{H_y} Y(h(x) - y(x,t) - z(x,t)) - ey(x,t), \tag{3}$$

$$\frac{dz}{dt}(x,t) = c_z \frac{g_z(x)}{H_z} Z(h(x) - y(x,t) - z(x,t)) - ez(x,t). \tag{4}$$

For *Cephalotes*, defense of nest cavities has driven the evolution of soldier castes with specialized head morphology for entrance blocking. For the origin of castes, therefore, we need to extend the above model to include such defense.

When colonies of phenotype 1 try to overtake a nest of width x inhabitated by a colony of phenotype 2, then colony 1 wins with a defense probability $d_{zy}(x)$. We assume that $d_{yz}(x) = 1 - d_{zy}(x)$ and that resident colonies do not have a 'home advantage': a colony of the same phenotype evicts a conspecific that currently lives in a nest cavity with probability of $\frac{1}{2}$. (Assuming such a home advantage instead would imply that the growth rate (invasion fitness) of resident populations at steady state would not be zero.)

Including this last ingredient gives

$$\begin{aligned}
\frac{dy}{dt}(x,t) &= c_y \frac{g_y(x)}{H_y} Y[d_{zy}(x)z(x,t) + h(x) - y(x,t) - z(x,t)] \\
&\quad - c_z \frac{g_z(x)}{H_z} Z d_{yz}(x)y(x,t) - ey(x,t), \\
\frac{dz}{dt}(x,t) &= c_z \frac{g_z(x)}{H_z} Z[d_{yz}(x)y(x,t) + h(x) - y(x,t) - z(x,t)] \\
&\quad - c_y \frac{g_y(x)}{H_y} Y d_{zy}(x)z(x,t) - ez(x,t).
\end{aligned}$$

which is equivalent to

$$\begin{aligned}\frac{dy}{dt}(x,t) = {} & c_y\frac{g_y(x)}{H_y}Y[h(x)-y(x,t)-d_{yz}(x)z(x,t)] \\ & - c_z\frac{g_z(x)}{H_z}Zd_{yz}(x)y(x,t)-ey(x,t), \qquad (5)\\ \frac{dz}{dt}(x,t) = {} & c_z\frac{g_z(x)}{H_z}Z[h(x)-d_{zy}(x)y(x,t)-z(x,t)] \\ & - c_y\frac{g_y(x)}{H_y}Yd_{zy}(x)z(x,t)-ez(x,t), \qquad (6)\end{aligned}$$

since $d_{yz}(x)+d_{zy}(x)=1$. In what follows, we will distinguish different phenotypes by trait vectors $\mathbf{t}$ (for phenotype 1, fraction y), and $\mathbf{t}'$ (for phenotype 2, fraction z). Written in terms of these traits, the above equations are written as

$$\begin{aligned}\frac{dy}{dt}(x,t) = {} & c(\mathbf{t})\frac{g(x;\mathbf{t})}{H(\mathbf{t})}Y[h(x)-y(x,t)-d(x;\mathbf{t},\mathbf{t}')z(x,t)] \\ & - c(\mathbf{t}')\frac{g(x;\mathbf{t}')}{H(\mathbf{t}')}Zd(x;\mathbf{t},\mathbf{t}')y(x,t)-ey(x,t),\\ \frac{dz}{dt}(x,t) = {} & c(\mathbf{t}')\frac{g(x;\mathbf{t}')}{H(\mathbf{t}')}Z[h(x)-d(x;\mathbf{t}',\mathbf{t})y(x,t)-z(x,t)] \\ & - c(\mathbf{t})\frac{g(x;\mathbf{t})}{H(\mathbf{t})}Yd(x;\mathbf{t}',\mathbf{t})z(x,t)-ez(x,t).\end{aligned}$$

2.3. **Parameter mapping.** In AD models, one needs to specify how the ecological parameters, such as colonization rate, preference and defense, are determined by the traits. To distinguish monomorphic colonies, defined here simply as colonies with workers but no distinct soldier, from ones with castes, we describe colony size distributions by three traits, m, s and r. Trait m describes the mean of the smaller ants, $s \geq 0$ stands for the distance between the mean of the smaller and the larger soldier ants, and r the fractional investment in larger ants (see Figure 3). Since nest cavities are well-defended by ants that have the right sized head disk, the size distribution of ants in a colony is described in x. Let $\mathbf{t}=(m,s,r)$ be the trait vector, and

$$b(x;\mathbf{t}) = (1-r)\mathcal{N}(x,m,\sigma) + r\mathcal{N}\left(x, m+\frac{s}{2},\sigma\right)$$

be the size distribution of ants with head width x. Here $\mathcal{N}(x,m,\sigma)$ is a normal distribution with mean m and standard deviation σ. This standard deviation is taken fixed equal to 1 throughout, and is not considered to be part of the trait vector $\mathbf{t}$. For small s this distribution is not bimodal. We also make the following observation, set aside as a remark for future reference.

Remark 2.1. *If $r=0$, then for a given m, the size distribution specified by $(m,s,0)$ is identical for every s.*

We divide the total size distribution into small ants b_s and large ants b_l, but we defer a precise definition until later. Only small ants are assumed to contribute to reproduction and colonization; large ants contribute to defense. The colonisation parameter c is taken to be equal to the total contribution to reproduction by all the small ants.

To introduce a tension between reproduction and defense, we assume that ants contribute optimally to colonization when they have size B, but less so when they are either larger than B or smaller, by setting

$$c(\mathbf{t}) = A \int b_s(x;\mathbf{t})\mathcal{N}(x, B, 0.5)dx.$$

A is a scalar; the standard deviation 0.5 is chosen arbitrarily, but should be chosen less than that of the nest size distribution. Since defense strength for a nest with entrance width x is directly related to having ants with head disks of that size, we propose that a colony from phenotype 1 with $b_l(x;\mathbf{t})$ large ants is able to defend successfully a nest of size x from attack by $b_l(x;\mathbf{t}')$ ants from phenotype 2 with probability

$$d_{yz}(x) = d(x;\mathbf{t},\mathbf{t}') = D(\epsilon(b_l(x;\mathbf{t}) - b_l(x;\mathbf{t}'))).$$

The main assumption we make is that colony phenotype 1 has a greater probability to win a contest over a nest of size x from phenotype 2 if the first has more large ants of that same size than the second. Function $D(\cdot)$ should be increasing, between 0 and 1, and antisymmetric around 0. We examine two choices for D,

$$D_1(x) = \frac{1}{2}(1 + \tanh(x)), \quad D_2(x) = \frac{1}{2}(1 + \arctan(2x)).$$

Parameter ϵ measures the strength of the defense response.

Depending on the presence or absence of castes, *Cephalotes* species show different preferences for nests of different widths (Powell, 2008, 2009). All species have a certain minimal nest width they prefer, given approximately by the head size of the largest ant in the colony. Monomorphic species have an entrance preference many times larger than the head size of the largest ant, and often in the range of three times the head size of one ant (Powell, 2008). Colonies with well-developed castes prefer a much narrower range of nest entrance widths, one that is more in line with the head size of the soldiers. To implement this, we introduce a function $\lambda(s,r)$ which measure the extent of caste specialization of a colony. For fixed s, this function should be symmetric around $r = \frac{1}{2}$, be zero at $r = 0$ and $r = 1$ (investing all biomass in soldier ants also constitutes a monomorphic colony) and be increasing-decreasing. We try two implementations,

$$\lambda_1(r,s) = \left(1 - e^{-\frac{3rs}{\sigma}}\right)\left(1 - e^{-\frac{3(1-rs)}{\sigma}}\right), \quad \lambda_2(r,s) = \left(\frac{r}{\frac{\sigma}{2s} + r}\right)\left(\frac{1-r}{\frac{\sigma}{2s} + (1-r)}\right)$$

The factor 3 in λ_1 and 2 in λ_2 are such that caste specialization is pronounced when $s \approx 3\sigma$.

The preference function $g(x)$ is now defined by

$$g(x) = \mathcal{N}(x, P, \pi),$$

where P and π interpolate between the mean preference and it standard deviation between completely monomorphic ($\lambda = 0$) and maximally specialized $\lambda = 1$ colonies,

$$P = \lambda\left(m + \frac{s}{2}\right) + (1-\lambda)3m,$$
$$\pi = \lambda\sigma + (1-\lambda)3\sigma.$$

Finally, we define the size distributions of small and large ants, by introducing a transition function $v(x;\mathbf{t})$ that indicates the propensity for an ant of head size x to contribute to colonization or defense, and thus be termed "small" or "large". This function should increase from 0 to 1, and $v(m + \frac{s}{4}; m, s, \sigma) = \frac{1}{2}$ (the half way point should occur in the middle between mean m and mean $m+\frac{s}{2}$). We try two implementations,

$$\begin{aligned} v_1(x;\mathbf{t}) &= \frac{1}{2}\left(1+\tanh\left(2\sigma\left(x-m-\frac{s}{4}\right)\right)\right), \\ v_2(x;\mathbf{t}) &= \frac{1}{2}\left(1+\arctan\left(4\sigma\left(x-m-\frac{s}{4}\right)\right)\right). \end{aligned}$$

The steepness of the transition should depend on the width of the normal distributions, which scale with σ, and this is taken into account by the factor 2σ and 4σ, respectively. Then we define the size distributions for small and large ants by

$$b_s(x) = (1-\lambda v(x))b(x), \quad b_l(x) = \lambda v(x) b(x).$$

Figure 4 gives some examples of the ecological traits, both for a monomorphic colony and for one with a pronounced caste. All the parameters used in the mapping between traits and ecological parameters are collected in Table 2.

2.4. **The AD canonical equation.** In Adaptive Dynamics, the evolutionary change of traits over time is modeled using a decoupling of the ecological and evolutionary time scales. In the limit of infinitesimally small mutations, deterministic equations may be given that specify the expected evolutionary dynamics of the traits. These are called the AD canonical equations (Dieckmann and Law, 1996; Metz et al., 1996; Geritz et al., 1997, 1998), and will be specified forthwith.

Let us denote by $\phi(\mathbf{t},\mathbf{t}')$ the invasion exponent (i.e., the intrinsic exponential growth rate) of the invasive mutant with trait $\mathbf{t}'=(m',s',r')$ into a steady state resident population of phenotype $\mathbf{t}=(m,s,r)$, which has a nest occupancy $\bar{y}(x;\mathbf{t})$ and corresponding $\bar{Y}(\mathbf{t})$. Let $\mu(m)$ and $\tau^2(m)$ be the mean and variance in mutation step size, respectively, for trait m, and similarly for traits s and r. Then the evolutionary dynamics for three trait parameters m, s and r are specified by

$$\dot{m} = \frac{1}{2}\mu(m)\tau^2(m)\bar{Y}(\mathbf{t})\frac{\partial}{\partial m'}\phi(\mathbf{t},\mathbf{t}')|_{m'=m}, \tag{7}$$

$$\dot{s} = \frac{1}{2}\mu(s)\tau^2(s)\bar{Y}(\mathbf{t})\frac{\partial}{\partial s'}\phi(\mathbf{t},\mathbf{t}')|_{s'=s}, \tag{8}$$

$$\dot{r} = \frac{1}{2}\mu(r)\tau^2(r)\bar{Y}(\mathbf{t})\frac{\partial}{\partial r'}\phi(\mathbf{t},\mathbf{t}')|_{r'=r}. \tag{9}$$

Here the dot means a derivative with respect to evolutionary time. The evolution of two stably coexisting polymorphic colony phenotypes is given by analogous extension to a system of six equations. In the above formulation we have ignored the potential covariance of traits under mutation, since nothing is known about them. Note also that in all simulations of these equations, the mean and variance of the mutation process are unknown. This is not a significant problem if there is only one trait m, since then we would merely be rescaling evolutionary time by changing the value for $\mu(m)\tau^2(m)$. Here, this is not the case. We have no choice, however, but to take arbitrary values for these means and variances, which we take to be unity. We have experimented with other values of these means and variances, giving qualitatively very similar results.

Computing $\phi(\mathbf{t},\mathbf{t}')$ requires a linear stability analysis. This is not a trivial matter for the model under discussion, since there are no explicit expressions for the steady state profiles $\bar{y}(x)$ or for the mixed steady state profiles $(\bar{y}(x),\bar{z}(x))$. However, as detailed in the SI, implicit expressions may be given, and may be used in a separation of variables approach to find the invasion exponent. It turns out that $\phi(\mathbf{t},\mathbf{t}')$ solves an integral equation of the form

$$S(\mathbf{t},\mathbf{t}') := \int \frac{D(x;\mathbf{t},\mathbf{t}')}{C(x;\mathbf{t},\mathbf{t}') + \phi(\mathbf{t},\mathbf{t}')}\, dx = 1,$$

where $D(x;\mathbf{t},\mathbf{t}')$ and $C(x;\mathbf{t},\mathbf{t}')$ are given by

$$D(x;\mathbf{t},\mathbf{t}') := c(\mathbf{t}')\frac{g(x;\mathbf{t}')}{H(\mathbf{t}')}\big(h(x) - \bar{y}(x)d(x;\mathbf{t}',\mathbf{t})\big), \tag{10}$$

$$C(x;\mathbf{t},\mathbf{t}') := c(\mathbf{t})\frac{g(x;\mathbf{t})}{H(\mathbf{t})}d(x;\mathbf{t}',\mathbf{t})\bar{Y} + e. \tag{11}$$

Therefore, although the invasion exponent itself is not known explicitly, we know that

$$\operatorname{sign}\phi = \operatorname{sign}[T(\mathbf{t},\mathbf{t}') - 1] \tag{12}$$

where

$$T(\mathbf{t},\mathbf{t}') = \int \frac{D(x;\mathbf{t},\mathbf{t}')}{C(x;\mathbf{t},\mathbf{t}')}\, dx.$$

This integral is a *basic reproductive ratio* or *metapopulation capacity*, and the integrand balances colonization against extinction. Relation (12) is well-known and found in many models, including metapopulation models (Gyllenberg and Metz, 2001; Ovaskainen and Hanski, 2001).

As detailed in the SI, the change in the invasion exponent whilst varying parameter m is given by

$$\frac{\partial}{\partial m'}\phi(\mathbf{t},\mathbf{t}')\Big|_{m'=m} = \frac{\frac{\partial}{\partial m'}T(\mathbf{t},\mathbf{t}')\big|_{m'=m}}{\int \frac{D(x;\mathbf{t},\mathbf{t}')|_{m'=m}}{C^2(x;\mathbf{t},\mathbf{t}')|_{m'=m}}\, dx}.$$

The extension to higher dimensional trait space is entirely straightforward.

2.5. **Dynamics of the AD equations.** We make some preliminary remarks on the use of AD models, and the kind of dynamics they generate.

In many Adaptive Dynamics models, including this one, only a local stability analysis can be carried out, and it is not clear analytically what the long-term behaviour of the unstable solutions is. However, in most models, instability leads to substitution of the resident phenotype by the mutant phenotype (Dieckmann and Law, 1996). Indeed, this has been proved rigorously for a class of simple ODE models (Dercole and Rinaldi, 2008), but the current infinite-dimensional set of equations falls outside the scope of that class. We do not know if “invasion implies substitution” holds in our model. We have carried out extensive simulations of the ecological metapopulations model (also to check against simulated dynamics of the AD canonical equations), and these are all in accordance with the “invasion implies substitution” principle.

When defense strength ϵ is zero, the defense terms $d(x;\mathbf{t},\mathbf{t}')$ and $d(x;\mathbf{t}',\mathbf{t})$ are trivially 1/2, and castes do not enter in the model. The AD equation is hence only given by the evolutionary dynamics for m, the mean of the colony size distribution. In such a case, the evolutionary dynamics may be conveniently depicted using Pairwise-Invasibility-Plots (PIPs). Examples are given in Figure 6. Such a PIP illustrates graphically which of a given pair of residents and mutants invades the other. With the resident and mutant parameters as axes, the diagonal is thus neutral (resident and mutant are ecologically equivalent, so the invasion exponent ϕ is exactly 0 on the diagonal). If the area above the diagonal is dark, the mutant phenotype with a larger trait value will invade the resident phenotype and become the new resident. The AD dynamics will thus show an increase in the value of the trait. If the area below the diagonal is dark, the trait value will decrease in the AD dynamics. Often the AD dynamics will converge onto an evolutionary equilibrium. Depending on the local nature of the PIP at this equilibrium, it may instance be a terminal point or a branching point (for a full discussion, see (Dercole and Rinaldi, 2008), or (Diekmann, 2004) for an accessible first introduction to AD and PIPs).

When defense strength ϵ is positive, all three traits may change over evolutionary time. PIPs can now not be drawn, but the dynamics do generally converge onto a stable evolutionary equilibrium, and this again may or may not be a branching point.

2.6. **Description of simulation experiments.** The numerical experiments carried out with this model fall into two classes: establishing biologically reasonable dynamics, and simulating evolution of caste differentiation.

At the most basic level, we want the model to give plausible dynamics. We explore the metapopulation dynamics of the ecological model, which gives a first indication of the potential for coexistence of colony phenotypes. The most important biological phenomena we wish to see are

- when we vary the optimal worker size for colonization, B, the evolution of the traits should track this to keep reproduction at optimal levels;
- if defense strength ϵ goes up, investment in larger ants should become more viable;
- when we increase the width of preference functions, there should be less room for a colony phenotype with developed castes to coexist next to a monomorphic one (and evolution of such defensive phenotypes may thus be hindered by a simple lack of resources not monopolized by the resident in the evolutionary equilibrium).

Secondly, and most importantly, we want to know if the AD model shows evolutionary branching, and whether castes develop, before or after branching.

In this paper, we are chiefly interested in the interplay between ecological interactions, branching and caste differentiation. The main idea we wish to test theoretically is whether sustained disruptive selection may give rise to a novel caste of larger ants. However, the above setup does not preclude ecological branching in monomorphic colonies (colonies with a uniform worker size distribution), in which preferences for different parts of the resource distribution evolve. Therefore, we will first examine the simpler model (3)–(4), to see if such branching events take place under reasonable assumptions. After that, defense will be included and we will study the evolution of caste formation in the extended model (5)–(6). This latter model is more difficult to analyze, given the additional interactions between defense on the one hand, and colonization and preference on the other.

The details of the numerical implementation of the simulations may be found in the SI.

3. Results

3.1. **Ecological (metapopulation) dynamics.** Colonies with different phenotypes often coexist (Figures S1, S2). With increasing caste differentiation, the preference becomes narrower and defense more pronounced. This results in a narrow size range of suitable nests that are inhabited by the caste-bearing phenotype. Nest occupation by two different colony phenotypes may show overlap (Figure S1) when preferences of both phenotypes overlap. In this case, defense of nests with small nest entrances is quite pronounced, but it is not in line with nest preferences. As castes become more pronounced, the two phenotypes show more exclusive use of nest resources (Figure S2). This coexistence, of course, does not yet show that such a situation may be arrived at by branching from an evolutionary equilibrium. This will be discussed below.

3.2. **Evolutionary dynamics.** The first test of plausibility of this model is to see that evolutionary dynamics show a sensitivity to B, the worker size at which the colonization rate c_y is optimized. Starting at a point with no caste, $\mathbf{t} = (m, 0, 0)$, $m \neq B$, the evolutionary history indeed reflects this (Figure S3).

To understand the AD dynamics further, we first recall Remark 2.1, and note that the change from $(m, 0, 0)$ to (m, s, r), with r small and s positive (but not necessarily small) is continuous when seen from the perspective of size distributions. In fact it reflects only a small change in phenotype of the larger ants.

Starting with a colony phenotype without castes, the AD dynamics for one phenotype invariably shows that castes do not emerge before the equilibrium is reached. Since this could be due to monomorphic phenotypes being ill-defined (see Remark 2.1), we have also tried to start the one-species AD dynamics with (m, s, r) for which r is small, but s is not small. In all trials, r quickly decreased, resulting in an equilibrium with m close to B, $r = 0$ and s the value at which the dynamics had arrived when r had vanished.

As a first conclusion, we found as a robust pattern: the emergence of a stable evolutionary equilbrium of the form $(\bar{m}, \bar{s}, 0)$ with $\bar{s} \geq 0$.

We have found strong evidence of branching in the *absence* of defensive castes. Setting defense strength $\epsilon = 0$, we can still find branching points, as evidenced by Figure 6b. The relative width of preferences versus nest size distribution seems to play an important role in the occurrence of this phenomenon. With fixed nest size distributions, narrower preference distributions promote branching points, and wider distributions preclude them. Analogously, wider resource distributions promote branching for fixed preference widths. The means of the colony size distribution diverge after branching, and remain positioned more or less symmetrically around the original value in the equilibrium (Figure 7). This indicates a tug-of-war between optimal worker sizes for reproduction and colonization, and distinct preferences to use available resources. As a result, there is still significant overlap in resource use by the two phenotypes at the new evolutionarily stable state.

With $\epsilon > 0$, castes stably emerge after branching (Figure 8), even if the equilibrium is not a branching point for the no-defense model. Predictably, larger ϵ (stronger defense) facilitates branching and the emergence of castes. We do find, however, that the value of s of the mutant phenotype that needs to be introduced right after branching must not be too small. In other words, a phenotype with a few larger soldier ants needs to be introduced in order for the branching to occur. As discussed previously, this is not in conflict with the assumption in AD that all mutations should be small. The small distribution of soldier ants needs to be introduced in the tail of the main distribution, not outside it. This still constitutes a small evolutionary change in the ant phenotypes, since the original phenotypes had some larger ants already.

The evolutionary dynamics of branching with caste formation differs markedly from that of two branching monomorphic phenotypes (cf. Figures 7B vs. 8D). The pronounced castes correspond with more specialized preferences, which coincide more and more with the nest sizes that are well-defended by soldier ants. As a result, we find the coexistence of a monomorphic phenotype together with one which develops a soldier caste. These two phenotypes differ strongly in their preferences, and they are practically mutually exclusive in their resource use. We have never observed two phenotypes with castes coexisting in our AD simulations. Nevertheless, we conjecture that they might be found if the model were extended to three species, or if different soldier morphotypes with different defensive capabilities are introduced. Species with different morphotypes are found within the *Cephalotes* lineage (De Andrade and Baroni Urbani, 1999; Powell, 2008).

The mapping from the trait space to the ecological ingredients (preference, colonization and defense) included choosing three explicit functions, $D_1(x)$ vs. $D_2(x)$, $\lambda_1(r, s)$ vs. $\lambda_2(r, s)$ and $v_1(x; \mathbf{t})$ vs. $v_2(x; \mathbf{t})$. The most extreme difference in dynamics is expected when all three functions are replaced by their counterparts. In Figure S4, the equivalent of Figure 8 (which use $D_1(x)$, $\lambda_1(r, s)$ and $v_1(x; \mathbf{t})$) is shown in which all three functions have been replaced with their alternatives $D_2(x)$, $\lambda_2(r, s)$ and $v_2(x; \mathbf{t})$. The results are qualitatively very similar.

4. DISCUSSION

This paper provides a new theoretical understanding of phenotypic diversification in social insects, by showing that castes may evolve as the result of sympatric competitive interactions. More specifically, the benefits gained by a novel phenotypic mutant, within the highly competitive context of defending shelter resources, can produce disruptive selection and subsequent branching. We have shown that new castes generally do not develop before branching, but may result from the competition over evolutionary time with monomorphic colonies with which they compete for nest resources. Even without soldiers defending resources, a simple correlation between mean worker size and mean resource preference is sufficient to cause branching. Adding defensive capabilities further amplifies this, and may indeed cause a non-branching evolutionary equilibrium to turn into a branching point. We thus find evidence that ecological specialization within a population may occur in the absence of the evolution of a specialized caste, but that caste evolution may go hand-in-hand with the use of a narrower range of resources.

4.1. **Caste evolution and ecological specialization.** The intimate relationship that we identify here between the evolution of morphological and ecological specialization in novel colony phenotypes is concordant with empirical data for the turtle ants. As already discussed, the use of an increasingly narrow range of entrance sizes used by turtle ants is associated with discrete transitions in the evolution of a specialized soldier caste (Powell, 2008). While our model was built to reflect turtle ant biology, this did not guarantee that adaptive dynamics would generate a morphologically and ecologically specialized novel colony phenotype. Our results, however, suggest that disruptive selection is indeed a viable mechanism for producing the empirical pattern of coupled morphological and ecological speciation. Notably, this is in opposition to classical theory, which predicts the evolution of additional castes with the broadening of a species' ecological niche (Oster and Wilson, 1978). So, what evidence is there to support the empirical pattern and our modeling result in other taxa? With reexamination of recent ant work, it seems that the evolution of a novel specialized caste may indeed often be coupled with ecological specialization along a key niche axis.

Across *Eciton* army ant species, the evolution of a morphologically specialized prey-transport caste is associated with specialization on prey types that are more awkward to handle (Powell and Franks, 2006, 2005). A high proportional representation in the diet of a certain class of prey item therefore appears to have selected for a specialized caste to deliver it efficiently to the nest. In an intriguing example, the seed-harvester ant *Pogonomyrmex badius* has been used to test directly the classical idea that niche expansion is responsible for caste evolution, but no support has been found (Ferster et al., 2006; Traniello and Beshers, 1991). This is an ant that, unlike other members of the genus, has a specialized seed-milling caste and takes a larger range of seed sizes than its relatives. Nevertheless, ecological specialization is best analysed as the response to distribution and predictability of the focal resource for the organism that consumes it (Irschick et al., 2005), not simply niche breadth. In light of the findings here, and as proposed previously (Powell, 2008), a proportional specialization on large seeds might therefore explain the evolution of the specialized seed miller, not the byproduct of an expanded overall niche that comes from adding larger seeds to the diet. Similarly, the convergent evolution of a second specialized soldier or milling caste in a small number of *Pheidole* ant species found exclusively in the Southwest USA and nearby areas of Mexico (Moreau, 2008) might be associated with the size of available seeds (Huang and Wheeler, 2011), or defense against a specialized army ant predator (Huang, 2010). *Pheidole* is a hyper-diverse genus otherwise characterized by a discrete worker caste and a single large-headed caste that may function as a soldier or seed miller (Wilson, 2003).

To summarize, while empirical data on the ecology of caste evolution remain generally scarce, these studies suggest that ecological specialization may be an important force in the evolution of specialized castes across the ants.

4.2. **Caste evolution and resource distributions.** Our model suggests that for a given resource preference range of the ants, an overall broadening of the resource base available in the environment can drive the production of new species with more specialized niches, and the evolution of a new specialized caste in some cases. Classical caste theory predicts that this kind of change in the prevailing environment might provide "ecological release" of a species, and thus one type of opportunity for niche expansion and subsequent caste proliferation (Oster and Wilson, 1978). As outlined above, our results strongly reject this proposed pattern. Nevertheless, a central premise of the ecological theory of adaptive radiation (reviewed in Schluter (2000)) is that "ecological opportunity", like that provided by an expanded resource base, initiates the accelerated production of ecologically divergent species. Our findings are highly consistent with this premise, and yield a prediction that is specific to the diversification of social insect lineages: greater resource availability within the evolutionary history of a lineage should be followed by accelerated production of species that are both more ecologically specialized and have a greater prevalence of specialized castes.

A phylogenetic comparative framework has been proposed as a powerful approach to studying the evolution of different components of trait specialization (Irschick et al., 2005). In addition, phylogenetic comparative approaches now exist to test for the predicted accelerated accumulation of divergent species following ecological opportunity (e.g. (Mahler et al., 2010; Frédérich et al., 2013)). Here, the turtle ants can provide a few more concrete examples as to how correlated ecological specialization and caste evolution might be seen in association with new ecological opportunity. We know that turtle ants are dependent on beetle-produced cavities (Creighton and Nutting, 1965; Creighton, 1963; De Andrade and Baroni Urbani, 1999; Powell, 2008). We could therefore test whether an increase in species accumulation and transitions in caste evolution are coincident with increases in cavity resource availability. Conceivably, increases in cavity resources could be associated with a transition in habitat use (e.g. (Price et al., 2014)), moving into geographic locations with underused cavity resources, or through the diversification of the beetles themselves. The phylogenetic comparative patterns associated with these possibilities are potentially testable in the turtle ants, as are generally similar scenarios in other taxa.

4.3. **Caste evolution and the developmental origin of soldiers.** While our model suggests that caste evolution emerges stably after a branching point under a range of conditions, we do see that the mutant colony phenotype that ignites the process cannot have soldiers that are too small. This has biological significance for considering the developmental origin of novel castes. In fact, our result would have been problematic for the classical hypothesis of how novel phenotypes evolve. The long held view is that they emerge from the small incremental expansion of the ancestral worker size range (Wilson, 1953; Oster and Wilson, 1978). However, recent work has suggested that novel castes are more likely to originate from "developmental mosaics" of the existing castes (Baroni Urbani, 1998; Molet et al., 2012, 2014). Metamorphosis in holometabolous insects is controlled by a series of pairs of imaginal discs distributed throughout the pupa's body. The developmental pathways switched on in these different discs then determines the overall adult form. The developmental mosaic hypothesis proposes that novel castes originate as mosaics of expression of gyne and worker phenotype across the different imaginal discs (Molet et al., 2012). The result is a novel adult form composed of parts that have largely been tested by evolution in the existing castes, and that can provide specialized functions because other life-sustaining tasks are performed by other members of the society. Mosaic-like reproductive castes seem to be widespread in ant evolution (Molet et al., 2012), and evidence is mounting that novel soldier phenotypes may often originate as mosaic-like inter-castes that approximate a gyne head on a worker body (Molet et al., 2014). Moreover, individuals that are developmental mosaic mutants are relatively common in colonies of many ant taxa, and survive and operate readily within the buffered social environment (Molet et al., 2012; AntWeb, 2015). This includes turtle ants, where full colony collections often reveal the presence of individuals with mosaic-like, blended caste traits (e.g., typical worker body with incompletely formed soldier head; Powell unpublished data). All considered, the kind of initial soldier size needed to kickstart stable caste differentiation in our model may be relatively straightforward, and perhaps even common, within the constraints of ant developmental biology.

4.4. **From branching to speciation.** The evolutionary dynamics resulting in the origin of a new soldier-bearing phenotype within a monomorphic population, focused on here, is the critical first step in ecological speciation, but it is not a true speciation event. This requires that the phenotypic divergence within the population is also associated with reproductive isolation (Schluter, 2000; Nosil, 2012). This is possible if the ecological traits under disruptive selection also generate assortative mating. Historically, "magic traits", defined as ecological traits under selection that are also directly involved in mating cues, have been seen as a likely rare occurrence, hence the name (Nosil, 2012). Nevertheless, recent work has made an important distinction between these "classic" magic traits and "automatic" magic traits (Servedio et al., 2011; Nosil, 2012). The idea behind automatic magic traits is that adaptive phenotypic divergence of ecological traits may frequently establish pre-mating reproductive isolation as an automatic byproduct (Servedio et al., 2011; Nosil, 2012). Known aspects of turtle ant biology suggest that divergent selection on worker sizes and associated entrance size preferences, as explored in this model, may have a number of cascading, automatic effects on mating cues.

Beetle cavities with smaller entrance holes tend to be in smaller diameter stems, more towards the terminal tips of tree crowns (Powell unpublished data). This makes intuitive sense because although small beetle species could potentially feed in and emerge from large stems, the greater nutritional needs of large beetle species would naturally exclude them from certain smaller size classes of stems. Given the demonstrated association between soldier size and entrance preferences in turtle ants (Powell, 2008, 2009), adaptive divergence in these traits among populations has natural spatial implications for the locations of the cavities they occupy. Critically, mounting evidence suggests that turtle ant virgin females (alate gynes) engage in female calling to males at or near the natal nest. Female calling involves the release of sex pheromones that draw in winged males to the point location of the calling females. Across ant species, this mating strategy is often associated with the production of small numbers of very large gynes, large robust males, localized dispersal behavior of gynes post-mating, spatial clumping of colonies, small colony size at reproductive maturity, and the prolonged release of sexuals instead of a mass-release (Hölldobler and Wilson, 1990; Boomsma et al., 2005; Peeters and Molet, 2010), all of which have been documented in turtle ants (Corn (1976); De Andrade and Baroni Urbani (1999); Powell (2009); Powell unpublished data). Any spatial segregation in cavity locations among populations, driven by divergent selection on ecological traits for cavity defense and selection, may therefore have profound effects on assortative mating. While these ideas are speculative at this stage, they provide a number of testable hypotheses about the spatial and temporal aspects of turtle ant mating biology. It may also be possible to incorporate any new empirical insights into assortative mating into future models. The AD canonical equation we have developed here is based on the assumption of clonal reproduction, as is common. Nevertheless, extending the AD framework to sexually reproducing species is possible (Dieckmann and Doebeli, 1999; Dieckmann et al., 2004), but requires that the evolutionary dynamics are modeled using an individual-based approach, at the expense of analytical tractability.

4.5. **Critique of the modeling approach, and expected results.** The model studied in this paper is intricate, but, in a certain sense, it is also minimal. To capture the evolution of traits in a meaningful manner, we have introduced first an ecological model in which different species compete for resources (nest space). Additionally, we have defined a mapping from the trait space to the ecological parameters in that first model. This was the most difficult step. Then, we have introduced the AD canonical equations that describe the evolution of the traits on an evolutionary timescale.

We have tried to keep the trait space as low-dimensional as possible, but three parameters seem to be the smallest number to distinguish unimodal from bimodal ant worker size distributions. Also the mapping from trait space to the ecological functions of defense, preference and colonization is kept as simple as possible, but simple it certainly is not. We definitely do not think ours is the only implementation of this mapping. For instance, it may well be reasonable to make defense strength ϵ an evolutionarily dynamic variable, mimicking the evolutionary transitions in distinct soldier morphotypes among *Cephalotes* species. Since this paper's goal was to show that sympatric ecological competition and ensuing disruptive selection is a viable mechanism for caste formation, there is clearly no interest in trying to find exactly where the boundaries lie in parameter space between the observed behaviors (branching versus no branching, for example).

4.6. **Outlook for caste theory.** Our model provides the first exploration of how resource competition in sympatry might drive phenotypic divergence, caste evolution, and potentially ultimately speciation. It remains to be seen to what extent this model may be generalized to other well-known taxa with specialized castes, like *Eciton*, *Pogonomyrmex* and *Pheidole*. For instance, in *Eciton* the resource base shared by different army ant species is much more dynamic than the nest resource is for turtle ants. We have used a metapopulation approach for *Cephalotes*, but a more common Volterra competition model of some kind might be more reasonable for *Eciton*. Nevertheless, our general approach makes a conceptual shift to considering how phenotypic diversification in complex social taxa might be explicitly coupled with the process of ecological speciation, and adaptive lineage diversification more generally. This provides a potentially valuable and alternative perspective to classical thinking on caste evolution, which explicitly considers the process of evolutionary branching. At the most general level, our model can be seen as a critical step in bridging the historical divide between the development of mainstream evolutionary theory on phenotypic diversification and the study of this process on complex social taxa. We suggest that continued efforts to unite the study of phenotypic diversification across different levels of biological complexity are likely to provide valuable tests of the general processes thought to drive adaptive evolution.

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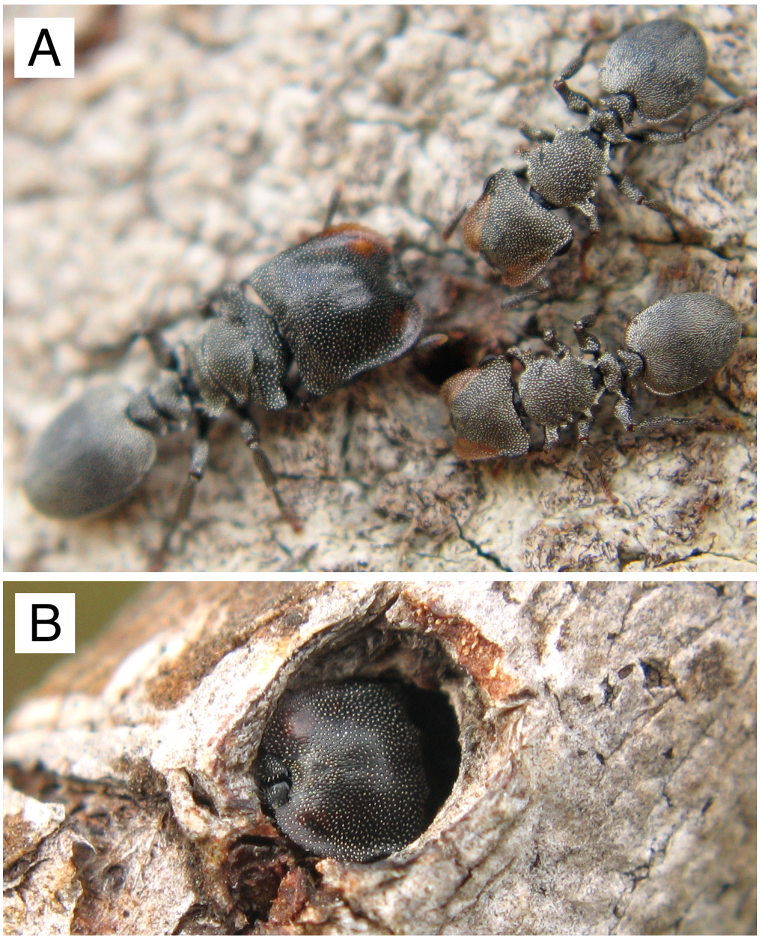

Figure 1. A soldier (left) and two workers (right) of the turtle ant *Cephalotes depressus* (A), and a soldier blocking the entrance of a nest cavity occupied by its colony (B). Photos by Scott Powell.

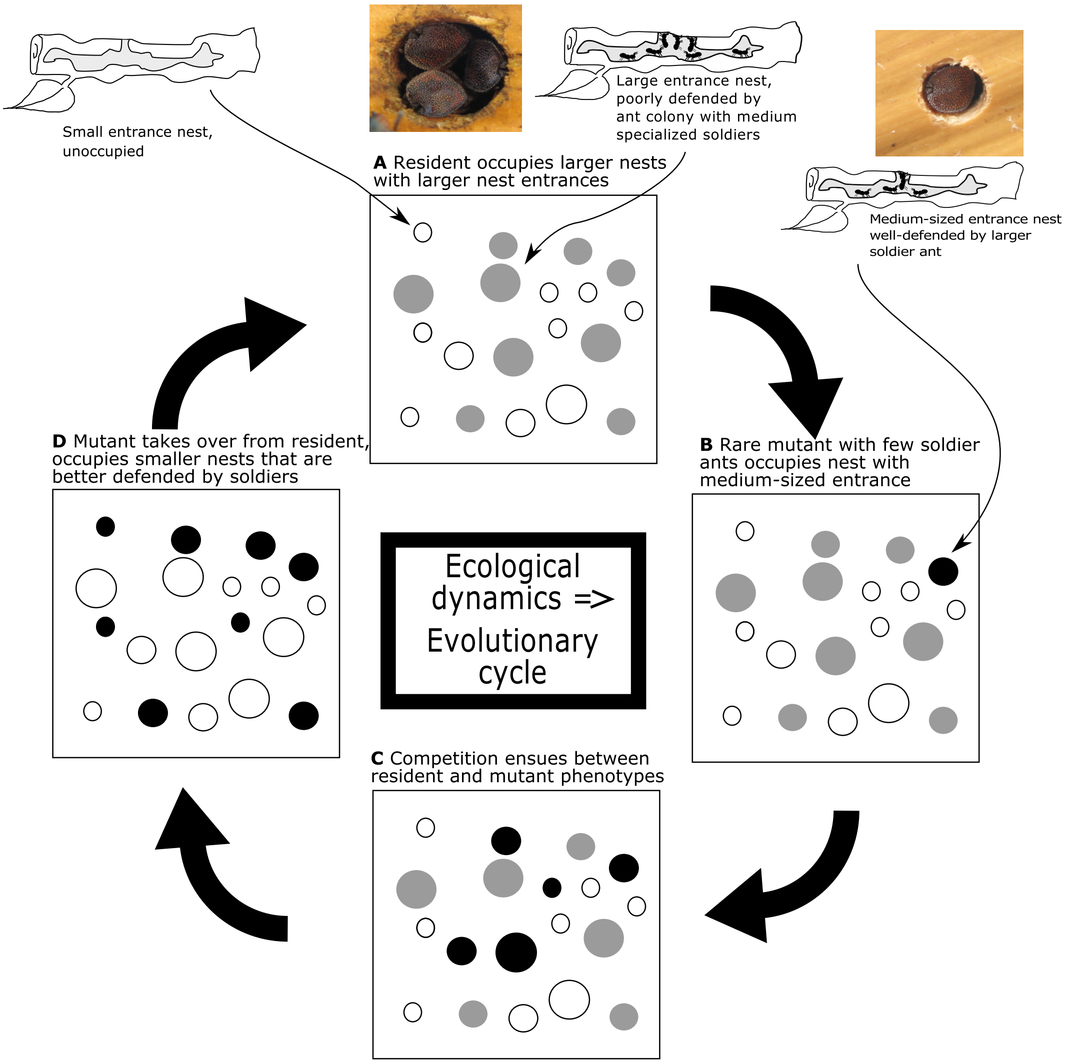

Figure 2. Cartoon-like illustration of the ecological dynamics in a single evolutionary cycle, explaining the basic logic of the model. (A) a resident phenotype with a few soldiers occupies nests of varying, mostly larger, entrance widths. The colony has a preference for larger nests (which are more abundant), but cannot defend these very well. (B) a colony mutates, and has larger soldier ants. Preference of this colony is for slightly smaller nests, which can be defended better. (C) Competition ensues between the resident and mutant colony phenotypes. (D) In this example, the mutant overtakes the resident and becomes the new resident. The cycle then recommences. Photos by Scott Powell.

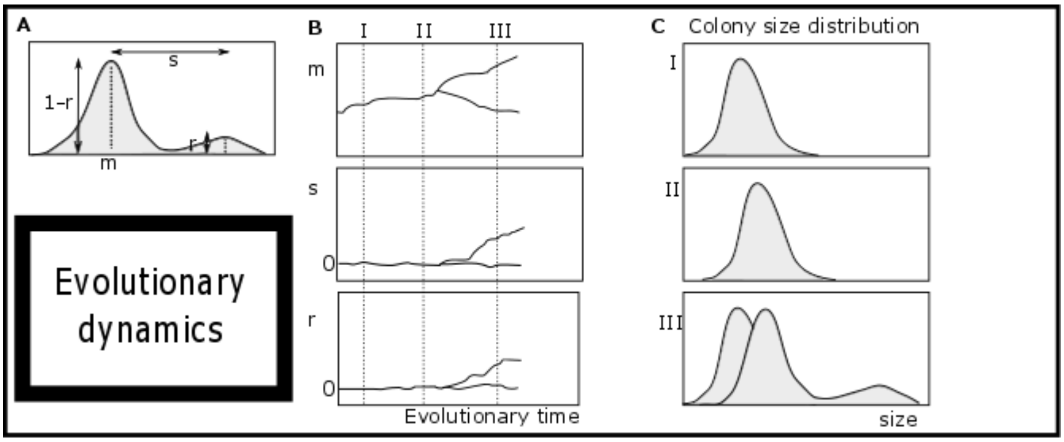

Figure 3. Schematic evolutionary dynamics. (A) Ant worker size distributions are speficied by three parameters, m (the mean of the smaller ant size), s (the distance between the means of smaller and larger ant sizes, and r, the fraction of biomass invested in larger ants. (B) Example (schematic) evolutionary dynamics of the three traits, m, s and r. Until branching occurs, there is no caste proliferation. After branching, one phenotype develops castes (r and s positive), the other does not. (C) Example worker size distributions at corresponding evolutionary time moments in (B).

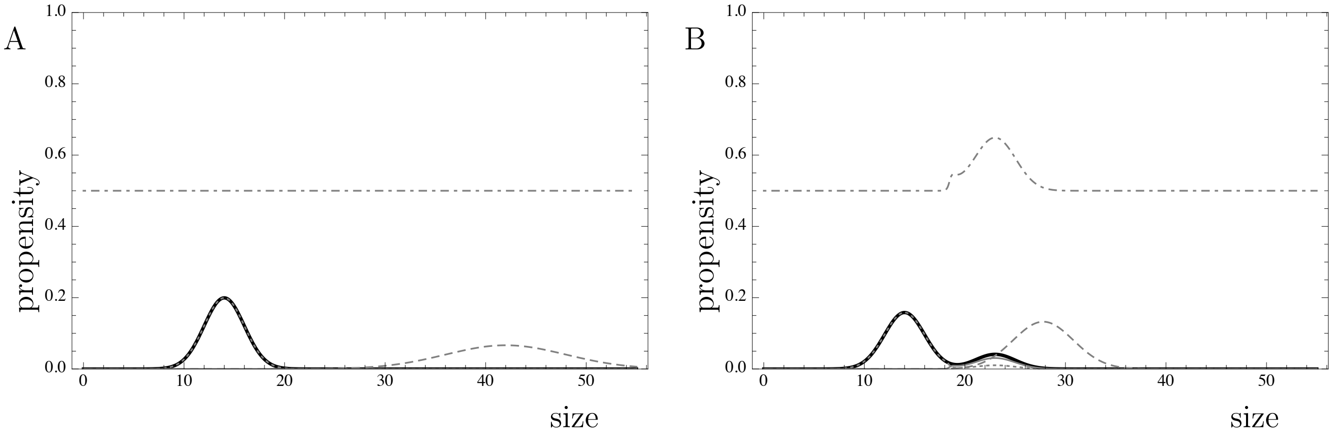

Figure 4. Two example choices for the important functions that define a species' traits. Black thick line: total biomass b; light gray: large ants b_l, dashed gray: preference; dashed-dotted line: defense d (against a monomorphic colony, i.e., its $b_l(x) = 0$); Parameter choices for figure A: $m = 14$, $s = 0$, $r = 0$, $\sigma = 1$, defense strength $\epsilon = 0$. For figure B, parameters are the same except $s = 3$, $r = 0.3$. The left figure shows a species without a caste with specific abilities to defend nest sizes. The right figure shows a species with a pronounced soldier caste, good defensive abilities and preferences that match the nest sizes that may be defended.

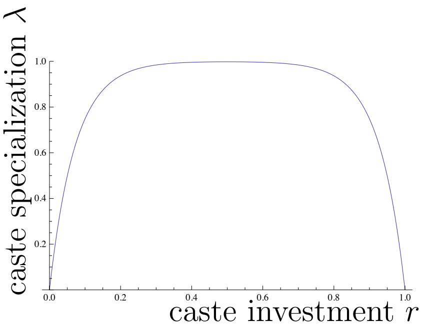

FIGURE 5. Example caste specialization function $\lambda_1(s, r)$ as a function of r. In this example, $s = 4.6$. Note that λ_1 is symmetric around $r = \frac{1}{2}$, and is maximal there. Since the value of s is quite high, even a small bit of biomass invested in larger ants ($r > 0$ small) results in a high caste specialization.

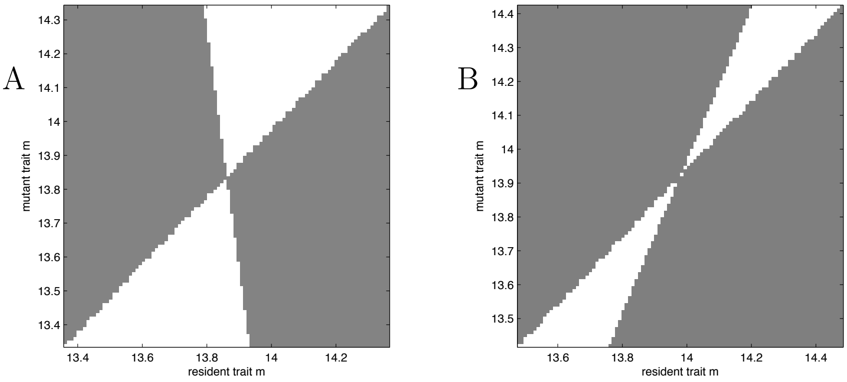

FIGURE 6. Branching in the absence of defense, illustrated using Pairwise-Invasibility-Plots (PIPs). (A): a relatively wide preference width ($\sigma = 4.5$) (relative to the nest size distribution) ensures that the evolutionary equilibrium is convergence stable. (B): Narrowing the preference ($\sigma = 1$) induces the occurrence of a branching point. Parameters common to both figures are $B = 14$, $\epsilon = 0$, $n = 100$.

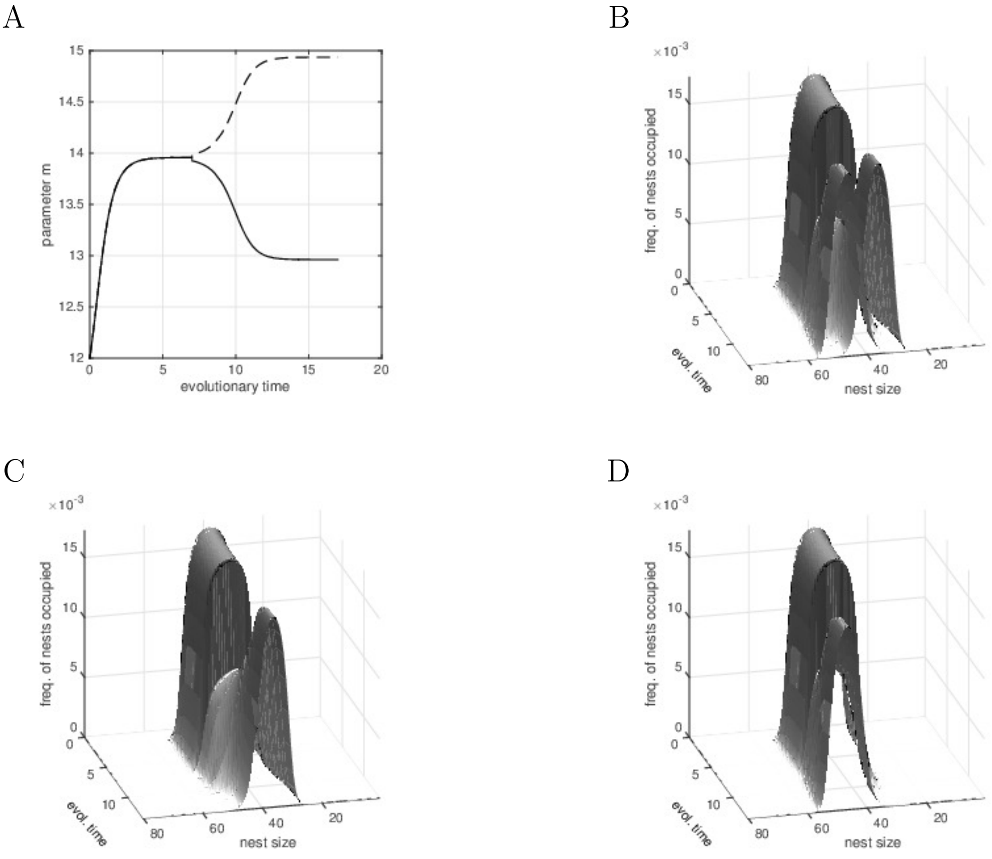

FIGURE 7. Branching in the absence of defense. Evolutionary dynamics for defense strength $\epsilon = 0$, with parameters as in Figure 6B, so that the evolutionary equilibrium is a branching point. (A): evolution of parameters m; (B): nest occupancy of both phenotypes; (C): nest occupancy of phenotype A only; (D): nest occupancy of phenotype B only. Phenotypes A and B are one and the same phenotype for $t \in [0, 10]$. Note that at the branching point, the branching phenotypes are ecologically nearly identical, and thus share the resources nearly equally, resulting in a sudden drop in nest use. Also note that the branching phenotypes progressively use more exclusive nest resources.

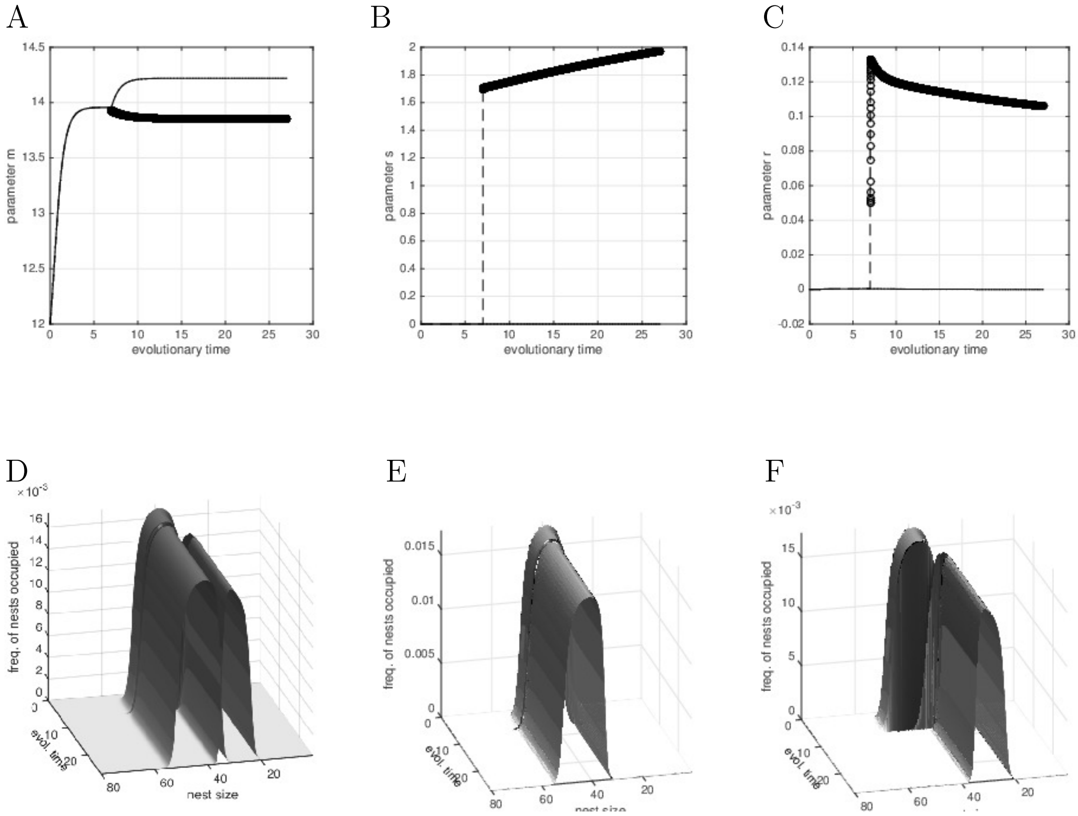

FIGURE 8. Defense facilitates branching, using $D_1(x)$ for defense, $\lambda_1(r,s)$ for the caste specialization function, and $v_1(x,\mathbf{t})$ for the transition function for small and large ants. . Evolutionary dynamics for defense strength $\epsilon = 10$, where parameters are chosen such that the $\epsilon = 0$ model is *not* a branching point. For positive ϵ, the evolutionary equilibrium is a branching point, and distinct castes develop. (A)-(C): evolution of parameters m, s and r, respectively. (D)-(F): nest occupancy of both phenotypes (D), phenotype A only (E) and phenotype B only (F). Phenotypes A and B are one and the same phenotype for $t \in [0, 20]$. Note that at the branching point, a distinct jump in s is taken, but that the jump in r is relatively small (relative to its final value), see Remark 5.1 in the Online Appendix. Also keep in mind that phenotype B thus develops a soldier caste and occupies a distinct nest size range in correspondence with its new preference and defensive abilities. Parameters are $B = 14$, $\sigma = 3.5$, $\epsilon = 10$, $n = 100$.

Model ingredient	**Variable**
Resource distribution	$h(x)$
Preference profile	$g_y(x)$ / $g(x;\mathbf{t})$
Defense probability	$d_{zy}(x)$ / $d(x;\mathbf{t},\mathbf{t}')$
Colonization rate	c_y / $c(\mathbf{t})$
Worker biomass distribution	$b(x;\mathbf{t})$
Small workers biomass distribution	$b_s(x;\mathbf{t})$
Large workers biomass distribution	$b_l(x;\mathbf{t})$
Caste specialization	$\lambda(s,r)$
Size transition function	$v(x;\mathbf{t})$

TABLE 1. Model ingredients, highlighting also the different types of notations used in the ecological model $(g_y(x), c_y, d_{yz})$ or using trait vectors $\mathbf{t}$ and $\mathbf{t}'$.

Parameter	**Description**	**Value/Range**
B	Ant size at which colonization rate is optimal	12, 14
σ	standard deviation of ant size distributions	1
ϵ	strength of defense response	0, 10
A	prefactor for colonization rate	100
σ_h	standard deviation of nest size distribution	4
w	mean size of nest entrance	20
e	rate at which nests are abandoned	1
m	mean worker size of monomorphic colony	dynamic
s	distance between biomass peaks of the worker size distribution	dynamic
r	fraction of total biomass allocated to soldier caste	dynamic
n	number of different nest sizes, used in solving ODE model numerically	100, 200

TABLE 2. Parameter settings used in this paper. Parameter are grouped as: parameters whose effect on the evolution is studied; fixed model parameters; evolutionary trait parameters; numerical parameters used to carry out the simulations.

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SUPPLEMENTARY INFORMATION TO DISRUPTIVE SELECTION AS A DRIVER OF EVOLUTIONARY BRANCHING AND CASTE EVOLUTION IN SOCIAL INSECTS

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1. ODE results: Steady states

We restate the full ecological model,

$$\begin{aligned}\frac{dy}{dt}(x,t) &= c_y\frac{g_y(x)}{H_y}Y[h(x)-y(x,t)-d_{yz}(x)z(x,t)]\\ &\quad - c_z\frac{g_z(x)}{H_z}Zd_{yz}(x)y(x,t)-ey(x,t), \qquad (1)\\ \frac{dz}{dt}(x,t) &= c_z\frac{g_z(x)}{H_z}Z[h(x)-d_{zy}(x)y(x,t)-z(x,t)]\\ &\quad - c_y\frac{g_y(x)}{H_y}Yd_{zy}(x)z(x,t)-ez(x,t). \qquad (2)\end{aligned}$$

To be able to simulate the AD canonical equations, we need to have information about two main objects:

- the steady state solutions of the ecological model (1)–(2), both for the two phenotype model (with one resident, one mutant) and for the three phenotype model (with two residents and one mutant);
- the basic reproductive ratio that is used whenever we need to find the derivative of the invasion fitness.

1.1. **One resident phenotype: generalist and specialist equilibria.** It is easy to find the steady state distribution for a generalist phenotype 1, in the absence of phenotype 2. Set $g_y = 1$, $z = 0$, and $\eta = e/c_y$. Then, integrating the first equation at steady state over x, we find

$$0 = \int \frac{Y}{H}(h(x)-y(x))\,dx - \eta\int y(x)\,dx,$$

so that

$$0 = \frac{Y}{H}(H-Y) - \eta Y$$

which has as nontrivial solution $Y = H(1-\eta)$ (phenotype 1 occupies all but a fraction of η of the patches) if $\eta < 1$. From this we deduce that $y(x) = h(x)(1-\eta)$. We will denote such an equilibrium patch profile by $\bar{y}$, and the equilibrium total patch occupancy by $\bar{Y}$.

If $g_y \not\equiv 1$, it is in general impossible to find a closed expression for the steady state. However, it is possible to find an implicit expression which is still useful for numerical computations. Let us assume that we know the steady state value of $\bar{Y}$. Then we can simply solve the steady state equation for y treating $\bar{Y}$ as a parameter, and find

$$\bar{y}(x) = \frac{g_y(x)h(x)\bar{Y}}{g_y(x)\bar{Y} + \eta H_y}. \tag{3}$$

This is only a steady state if additionally we know that

$$\bar{Y} = \int \frac{g_y(x)h(x)\bar{Y}}{g_y(x)\bar{Y} + \eta H_y}\, dx, \tag{4}$$

or, equivalently,

$$1 = \int \frac{g_y(x)h(x)}{g_y(x)\bar{Y} + \eta H_y}\, dx. \tag{5}$$

For $\bar{Y}$ between its limit values 0 and 1, the right-hand side of (5) is strictly decreasing in $\bar{Y}$. Note that when $\bar{Y} = 1$,

$$\int \frac{g_y(x)h(x)}{g_y(x) + \eta H_y}\, dx \leq \left|\left|\frac{g(x)}{g(x) + \eta H_y}\right|\right|_\infty \int h(x)\, dx < \int h(x)\, dx = 1,$$

where $||.||_\infty$ denotes the sup norm. If we thus know that

$$\int \frac{g_y(x)h(x)}{\eta H_y}\, dx = \frac{1}{\eta} > 1,$$

then there exists a unique value of $\bar{Y}$ such that (4) is satisfied. The condition is thus $\eta < 1$, and this coincides with the existence of generalist equilibria. A phenotype must simply colonize at a faster rate than the rate at which it leaves patches—a common phenomenon in metapopulation models.

1.2. **Two resident phenotypes: mixed equilibria.** This implicit method may be extended to mixed equilibria $(\bar{y}(x), \bar{z}(x))$.

Equations (1) and (2) may be solved implicitly at steady state for given x, $\bar{Y}$ and $\bar{Z}$, to find

$$\bar{y}(x) = \frac{\hat{c}_y\bar{Y}h(x)(d_{zy}(x)(\hat{c}_y\bar{Y} + \hat{c}_z\bar{Z}) + e)}{(\hat{c}_y\bar{Y} + \hat{c}_z\bar{Z} + e)(d_{zy}(x)\hat{c}_y\bar{Y} + d_{yz}(x)\hat{c}_z\bar{Z} + e)}, \tag{6}$$

$$\bar{z}(x) = \frac{\hat{c}_z\bar{Z}h(x)(d_{yz}(x)(\hat{c}_y\bar{Y} + \hat{c}_z\bar{Z}) + e)}{(\hat{c}_y\bar{Y} + \hat{c}_z\bar{Z} + e)(d_{zy}(x)\hat{c}_y\bar{Y} + d_{yz}(x)\hat{c}_z\bar{Z} + e)}, \tag{7}$$

where

$$\hat{c}_y = c_y\frac{g_y(x)}{H_y}, \quad \hat{c}_z = c_z\frac{g_z(x)}{H_z}.$$

For these identies to be true equilibria, we need them additionally to satisfy

$$1 = \int \frac{\hat{c}_y h(x)(d_{zy}(x)(\hat{c}_y\bar{Y} + \hat{c}_z\bar{Z}) + e)}{(\hat{c}_y\bar{Y} + \hat{c}_z\bar{Z} + e)(d_{zy}(x)\hat{c}_y\bar{Y} + d_{yz}(x)\hat{c}_z\bar{Z} + e)}\, dx, \tag{8}$$

and

$$1 = \int \frac{\hat{c}_z h(x)(d_{yz}(x)(\hat{c}_y\bar{Y} + \hat{c}_z\bar{Z}) + e)}{(\hat{c}_y\bar{Y} + \hat{c}_z\bar{Z} + e)(d_{zy}(x)\hat{c}_y\bar{Y} + d_{yz}(x)\hat{c}_z\bar{Z} + e)}. \tag{9}$$

It is less clear under which general conditions these mixed steady states exist, but we can use this implicit form in numerics all the same.

2. ODE results: Linear stability analysis

The second major objective is to find the invasion exponent ϕ and corresponding basic reproductive ratio T used in the AD canonical equations. The invasion exponent $\phi(\mathbf{t}, \mathbf{t}')$ is the linear growth rate of the mutant with trait $\mathbf{t}'$ when introduced in small numbers in a steady state population of the resident with trait $\mathbf{t}$. Let us again start with the situation of one resident (phenotype 1, trait $\mathbf{t}$) and one mutant (phenotype 2, trait $\mathbf{t}'$).

The linearised equations for phenotype 2 around $(y, z) = (\bar{y}, 0)$ have the form

$$\frac{dz(x,t)}{dt} = D(x; \mathbf{t}, \mathbf{t}') \int z(x)\, dx - C(x; \mathbf{t}, \mathbf{t}') z(x),$$

where $D(x; \mathbf{t}, \mathbf{t}')$ and $C(x; \mathbf{t}, \mathbf{t}')$ are given by

$$D(x; \mathbf{t}, \mathbf{t}') := c(\mathbf{t}') \frac{g(x; \mathbf{t}')}{H(\mathbf{t}')} \big(h(x) - \bar{y}(x) d(x; \mathbf{t}', \mathbf{t}) \big), \tag{10}$$

$$C(x; \mathbf{t}, \mathbf{t}') := c(\mathbf{t}) \frac{g(x; \mathbf{t})}{H(\mathbf{t})} d(x; \mathbf{t}', \mathbf{t}) \bar{Y} + e. \tag{11}$$

The eigenvalue problem for $z(x,t)$ is given by testing for a solution $z(x,t) = \psi(t)\eta(x)$. Substituting this, we find that

$$\frac{\psi'(t)}{\psi(t)} = \frac{D(x; \mathbf{t}, \mathbf{t}')}{\eta(x)} \int \eta(x)\, dx - C(x; \mathbf{t}, \mathbf{t}').$$

The left hand side only depends on t, the right hand side only on x, so both must be a constant, ϕ, say. Hence $\psi(t) = c_0 e^{\phi t}$, and the sign of ϕ determines whether the solution $\eta(x)$ grows or declines in time. For this eigenfunction for a given ϕ, we have

$$\frac{\eta(x)}{\int \eta(x)\, dx} = \frac{D(x; \mathbf{t}, \mathbf{t}')}{\phi + C(x; \mathbf{t}, \mathbf{t}')}.$$

Integrating left and right over x, we find that ϕ needs to satisfy

$$S(\mathbf{t}, \mathbf{t}') := \int \frac{D(x; \mathbf{t}, \mathbf{t}')}{\phi + C(x; \mathbf{t}, \mathbf{t}')}\, dx = 1. \tag{12}$$

Hence, if

$$T(\mathbf{t}, \mathbf{t}') := \int \frac{D(x; \mathbf{t}, \mathbf{t}')}{C(x; \mathbf{t}, \mathbf{t}')}\, dx > 1 \tag{13}$$

then there exists a unique $\phi = \phi(\mathbf{t}, \mathbf{t}') > 0$ satisfying (12) and a corresponding eigenfunction $\eta(x)$ which grows in time. Written out in full, the basic reproductive ratio reads

$$T(\mathbf{t}, \mathbf{t}') = \frac{c(\mathbf{t}')}{c(\mathbf{t})} \frac{H(\mathbf{t})}{H(\mathbf{t}')} \int \frac{g(x; \mathbf{t}')(h(x) - \bar{y} d(x; \mathbf{t}', \mathbf{t}))}{g(x; \mathbf{t}) \bar{Y} d(x; \mathbf{t}', \mathbf{t}) + M} > 1, \tag{14}$$

where $M = \eta H(\mathbf{t}) = eH(\mathbf{t})/c(\mathbf{t})$.

A direct, but tedious, calculation using the implicit expression for the mixed steady state (3) shows that $T(\mathbf{t}, \mathbf{t}) = 1$: a resident phenotype cannot invade itself. This is biologically trivial (and is only true under the assumption that $d(x, \mathbf{t}, \mathbf{t}) = \frac{1}{2}$), but serves as a good benchmark for the simulations.

The generalisation to a mutant phenotype invading a mixed steady state of a pair of residents is entirely straightforward, and yields a very similar expression to (14). Again, the reproductive ratio is 1 if the mutant is equal to one of the two resident phenotypes.

Finally, we calculate how the derivative of $\phi(\mathbf{t}, \mathbf{t}')$ with respect to a mutant parameter m' relates to the derivative with respect to that same parameter of the basic reproductive ratio $T(\mathbf{t}, \mathbf{t}')$ at $m = m'$. Using that $\phi(\mathbf{t}, \mathbf{t}) = 0$, we find

$$\begin{aligned}
0 &= \frac{\partial}{\partial m'} S(\mathbf{t}, \mathbf{t}')\Big|_{m'=m} \\
&= \int \Big[\frac{(C(x;\mathbf{t},\mathbf{t}') + \phi(\mathbf{t},\mathbf{t}'))\frac{\partial}{\partial m'} D(x;\mathbf{t},\mathbf{t}')}{(C(x;\mathbf{t},\mathbf{t}') + \phi(\mathbf{t},\mathbf{t}'))^2} \Big]\Big]\Big|_{m'=m} \, dx \\
&\qquad - \int \frac{(\frac{\partial}{\partial m'}(C(x;\mathbf{t},\mathbf{t}') + \phi(\mathbf{t},\mathbf{t}'))D(x;\mathbf{t},\mathbf{t}')}{(C(x;\mathbf{t},\mathbf{t}') + \phi(\mathbf{t},\mathbf{t}'))^2} \Big]\Big]\Big|_{m'=m} \, dx \\
&= \int \Big[\frac{C(x;\mathbf{t},\mathbf{t}')|_{m'=m} \frac{\partial}{\partial m'} D(x;\mathbf{t},\mathbf{t}')|_{m'=m} - D(x;\mathbf{t},\mathbf{t}')|_{m'=m} \frac{\partial}{\partial m'} C(x;\mathbf{t},\mathbf{t}')|_{m'=m}}{C^2(x;\mathbf{t},\mathbf{t}')|_{m'=m}} \Big] \, dx \\
&\qquad - \int \Big[\frac{D(x;\mathbf{t},\mathbf{t}')|_{m'=m} \frac{\partial}{\partial m'} \phi(\mathbf{t},\mathbf{t}')|_{m'=m}}{C^2(x;\mathbf{t},\mathbf{t}')|_{m'=m}} \Big] \, dx \\
&= \frac{\partial}{\partial m'} T(\mathbf{t},\mathbf{t}')\Big|_{m'=m} - \frac{\partial}{\partial m'} \phi(\mathbf{t},\mathbf{t}')|_{m'=m} \int \frac{D(x;\mathbf{t},\mathbf{t})|_{m'=m}}{C^2(x;\mathbf{t},\mathbf{t})|_{m'=m}} \, dx.
\end{aligned}$$

We conclude

$$\frac{\partial}{\partial m'} \phi(\mathbf{t},\mathbf{t}')\Big|_{m'=m} = \frac{\frac{\partial}{\partial m'} T(\mathbf{t},\mathbf{t}')\Big|_{m'=m}}{\int \frac{D(x;\mathbf{t},\mathbf{t}')|_{m'=m}}{C^2(x;\mathbf{t},\mathbf{t}')|_{m'=m}} \, dx}.$$

3. IMPLEMENTATION OF SIMULATIONS

3.1. **The AD canonical equations.** To integrate the AD canonical equations, whether for one phenotype or for two coexisting phenotypes, we have to compute the matrix of partial derivatives of the invasion exponent with respect to the relevant variables. Rather than trying to find explicit closed expressions for these derivatives, we compute this Jacobi matrix numerically using the `numjac` function in Matlab. We have used the variable order `ode113` ODE solver in Matlab for all AD equation simulations.

After the one-phenotype AD equations are integrated, the dynamics arrive at an evolutionary equilibrium. To make sure that we have truly arrived at the equilibrium, we solve the right hand side of the AD equations algebraically, using the final value of the ODE integration as initial guess. Specifically, we use the Matlab function `fminsearch` on the sum of squares of the right hand side of the AD equations. For a steady state this sum of squares is zero. If the evolutionary equilibrium is not estimated carefully enough, it is not to be expected that two phenotypes will be able to coexist stably after we have switched to the two-phenotypes AD equations.

The evolutionary equilibrium now becomes the starting point of the two-phenotype AD equations. We make random mutations around the evolutionary equilibrium and each time compute the mixed steady state of the resulting pair of phenotypes. If, for a given mutation, the steady state profiles of both phenotypes occupy more than a fraction of 10^{-4} of total nest space at steady state, then we define this pair as the new coexisting pair of phenotypes and start integrating the two-phenotypes AD equations. If such a mutation cannot be found after 100 tries, the evolutionary equilibrium is termed not to be a potential branching point and is probably a stable evolutionary equilibrium.

3.1.1. *Numerically finding steady states.* To find specialist ecological steady states $\bar{y}(x)$ for a given trait vector, we use the implicit identity (3), together with the requirement (5). By varying Y we find the value for which (5) is met. For mixed ecological equilibria in

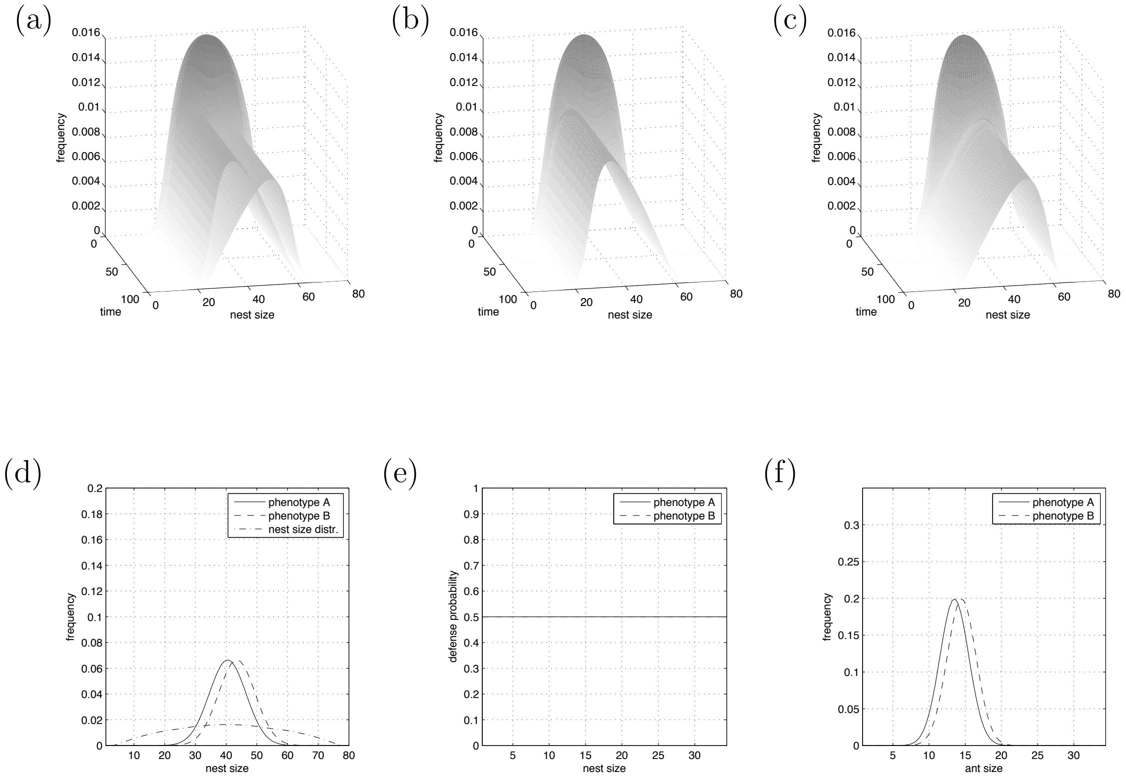

Figure S1. Example metapopulation dynamics for two competing phenotypes lacking castes. Parameters are $B = 14$, $A = 100$, $\epsilon = 0$, $n = 100$; for phenotype A, we set $(m, s, r) = (13.5, 0, 0)$, for phenotype B $(m, s, r) = (14.5, 0, 0)$. Initial conditions for each phenotype is set to the respective steady state nest occupancy distributions. The first row shows combined (a) nest occupancy dynamics, and for phenotype A (b) and B (c) alone. The second row shows preference (d), defense capabilities (e) (which are trivially 1/2 for both phenotypes) and worker size distributions (f) for both phenotypes. Note that the initial conditions widely overlap in nest occupancy, but that competition mediated by differences in preferences induces a mostly segregated nest occupancy.

which two phenotypes coexist at steady state, we have analogous implicit definitions (6) and (7), with corresponding additional integral conditions (8) and (9). Conditions (5), (8) and (9) are computed using Newton's method to find zeros of nonlinear equations.

The traits s and r have natural ranges of $[0, \infty)$ and $[0, 1]$, resp. At the boundary of the trait space ($s = 0$, $r = 0$ or both), we calculate the time derivatives in the usual manner, but set $\dot{s} = 0$ or $\dot{r} = 0$ if they happen to be negative.

Gyllenberg, M. and Metz, J. A. J. (2001). On fitness in structured metapopulation models. *J. Math. Biology*, 43:545–560.

Hanski, I. and Gaggiotti, O. E. (2004). *Ecology, genetics, and evolution of metapopulations.* Elsevier Academic Press.

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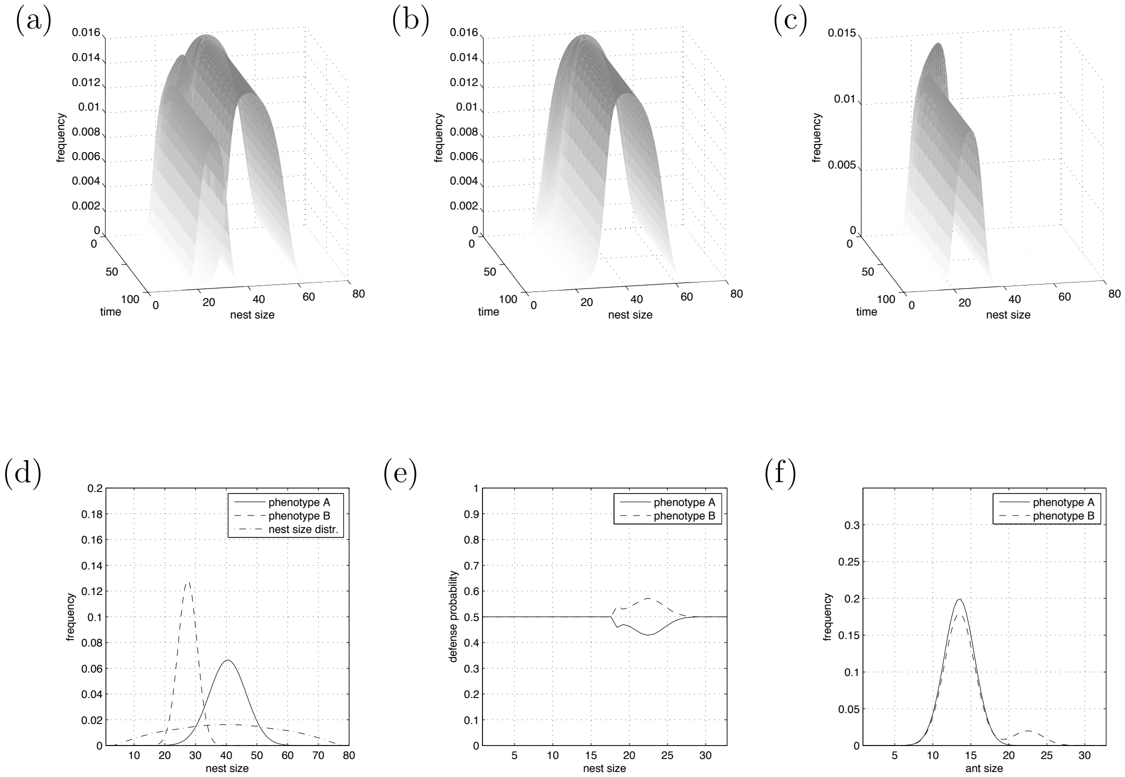

Figure S2. Example metapopulation dynamics for two competing phenotypes. See Figure S1 for details. Here we illustrate a phenotype A without a caste, and B with a caste. Parameters are as in Figure S1, except $(m, s, r) = (13.5, 0, 0)$ for phenotype A and $(m, s, r) = (13.5, 3, 0.1)$ for phenotype B.

Powell, S. (2008). Ecological specialization and the evolution of a specialized caste in *Cephalotes* ants. *Funct. Ecol.*, 22:902–911.

Powell, S. (2009). How ecology shapes caste evolution: linking resource use, morphology, performance and fitness in a superorganism. *J. Evol. Biology*, 22:1004–1013.

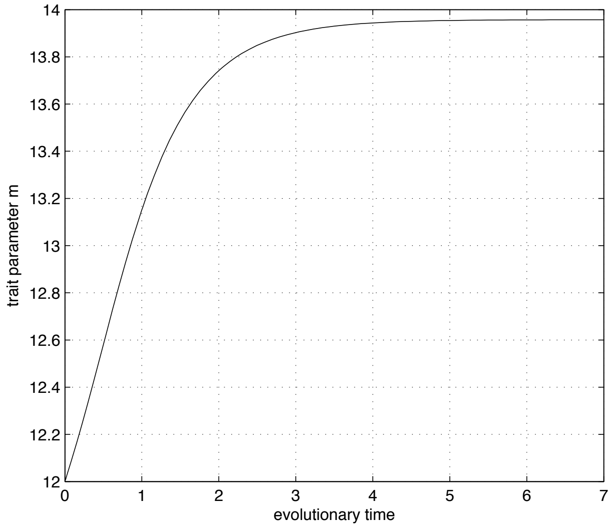

Figure S3. Evolutionary dynamics of trait variable m. In this illustration, the starting value of m was set far away from the optimal value, set by B. Note that the trait parameter evolves to near B. The equilibrium value of m does not need to coincide exactly with B. The The difference stems from various other components of the model, in particular the preference function, whose definition is independent of reproduction. Parameter values are $\epsilon = 0$, $A = 100$, $B = 14$, $\sigma = 1$.

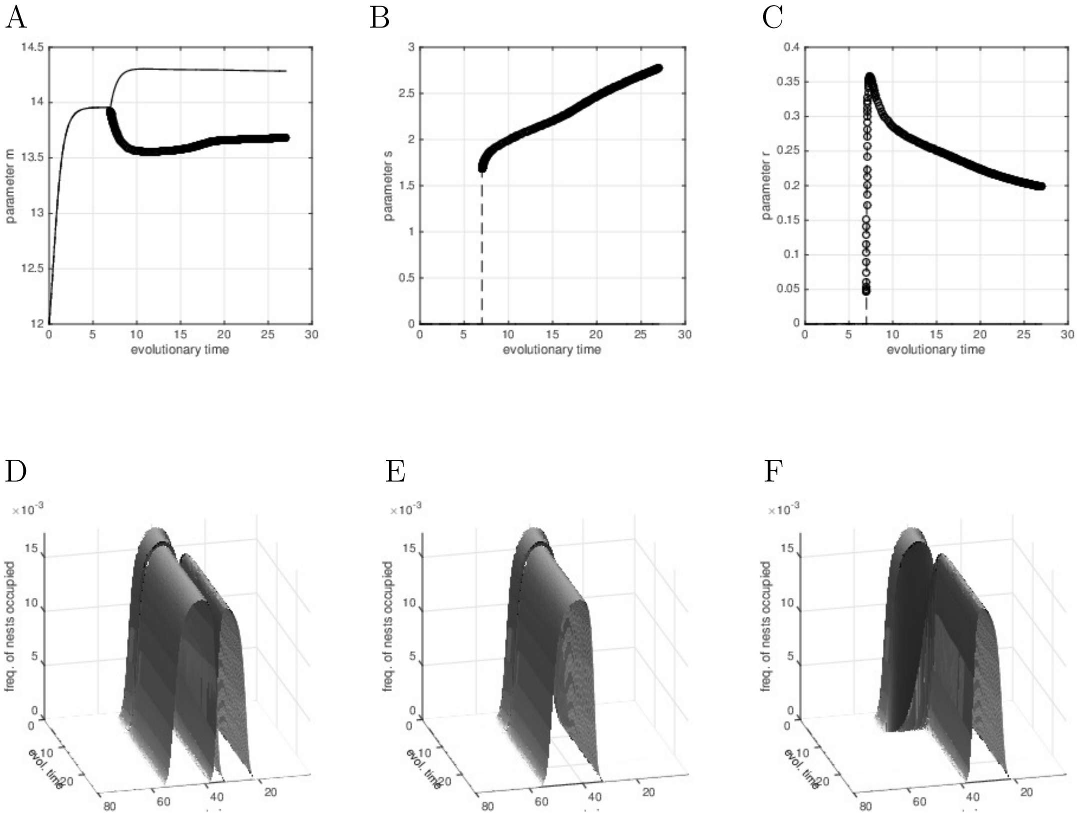

FIGURE S4. Defense facilitates branching, using $D_2(x)$ for defence, $\lambda_2(r, s)$ for the caste specialization function, and $v_2(x, \mathbf{t})$ for the transition function for small and large ants. All other parameters and settings are equal to those in Figure 8 in the main text.