**Supplementary file for**

**Range expansion drives the evolution of alternate reproductive strategies in invasive fire ants**

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Appendix A. Model design

Each simulation began with 50 colonies distributed randomly over 900 square meters within an arena (Figure 1a). The arena was 50 meters wide, bounded on its lower side, and unbounded in the upper direction. Starting colonies were assigned a colony size of 1,000 workers, approximating that of a young colony around 6 months old (Markin et al. 1973), and began with square territories measuring 3 by 3 meters. The vital parameters of all colonies (age, size, parent lineage, etc.), as well as their territory sizes and shapes, were maintained in a spatial polygons data frame (Pebesma & Bivand 2005, Bivand et al. 2013) throughout the simulation. We then simulated the growth, death, reproduction and dispersal of the colonies at monthly intervals for 25 years (300 time steps, ~4-8 generations, Tschinkel 2013). At each time step, the model progressed through a series of calculations outlined below.

*Step 1: Colony mortality*

Every month we calculated a survival probability for each colony based on its age and size (number of workers). Survival probability was determined from a combination of two functions. The first was an asymptotic function for monthly survival based on colony size:

*P*pop = 1 - e-0.002 \* (number of workers + 1,250)

This size-based function stipulated that smaller colonies were more likely to die, as they are more vulnerable to competitive interactions and demographic and environmental variability (Tschinkel 2013). The second function was based on the maximum longevity of queens and their limited supply of stored sperm, derived from a single mating early in life. This function was a flat power function that maintained a high but decreasing probability of survival before rapidly reducing to zero at about six years old (Tschinkel 1987):

*P*age = -2/1030 \* (age in months)16 + 1

The final survival probability was the product of the two functions *P*pop and *P*age. We applied this probability to each colony stochastically by comparing the calculated probability to a random value between 0 and 1. Colonies with probabilities greater than the randomly generated number survived. Colonies with probabilities lower than the randomly generated number lost their reproductive queen, became orphaned colonies, and began declining in size as the remaining workers died off (see *Step 2: Colony growth*).

*Step 2: Colony growth*

Every month we calculated the number of workers in each colony using a conditional function that applied different equations based on the current colony size and queen condition. Newly established colonies started with 40 workers, approximating the size of colonies just over one month old (Markin et al. 1973, Porter & Tschinkel 1986). In subsequent time steps we calculated the potential for colony growth using one of two equations. For small colonies with less than 2,500 workers we calculated growth according to a simple exponential model:

*P*init = 8.41 \* e0.972 \* (*t* + 1)

where *t* = current time in months (fit to data in Tschinkel 1988a and Booth & Dhami 2008). For larger colonies of at least 2,500 workers we used a logistic growth function (adapted from Tschinkel 1993):

*P*init = 165,000/(1 + 83 \* e-1.26/12 \* (*t* + 1))

where *t* = current time in months. Fire ant colony sizes fluctuate seasonally, such that they are at their largest in January and smallest in summer. To incorporate these seasonal oscillations, we augmented the colony growth equations with a cosine function (adapted from Tschinkel 1993):

*f* = cos(2 \* pi \* (*month* - 1)/12) \* 55,000

where *month* equals the current calendar month (1 to 12). Large colonies experience larger size fluctuations than do small colonies (Tschinkel 1993), so we adjusted the oscillations using a weighting factor (derived from Tschinkel 1993, by substituting a size-based function for the time-based term in the weighting factor on page 431):

*g* = 1,388,407 \* (number of workers)-1.1678667

The fluctuation for any given colony equaled the oscillation function *f* divided by the weighting factor *g*. We combined all the growth functions as follows to calculate the total potential colony size in any given time step:

*P*pot = *P*init + *f*/*g*

The colony’s new size was then provisionally updated in the spatial polygons data frame. A colony’s growth is related to its territory size, however, which determines the resources available to it (Tschinkel et al. 1995). We therefore adjusted potential colony growth in cases where a colony’s territory size was limiting (see *Step 3: Territory growth*).

Orphaned colonies whose queens had died (see *Step 1: Colony mortality*) declined in size instead of growing. We modeled this using a linear function that rendered the colony extinct within six months after queen death:

*Pt* = *P*t-1 - *P*t-1/(7 - *Td*)

where *Pt* is a colony’s size at a given time step and *Td* equals the number of months since queen death. We deleted orphaned colonies when they dropped below 100 workers in size.

*Step 3: Territory growth*

Fire ant colonies control exclusive territories from which they harvest the resources needed for growth, maintenance and reproduction, and aggressively defend their territories from neighboring colonies through worker-worker combat (Tschinkel et al. 1995, Tschinkel 2013). The result is a mosaic of irregularly shaped and non-overlapping territories that fill nearly all available habitat (Korzukhin & Porter 1994, Adams 1998). Simulating colony territory growth in a realistic manner was the most complicated element of the model, because we had to address the intrinsic capacity of each colony to expand based on the number of its workers, while accounting for limits on territory growth imposed by neighboring colonies.

The territory growth process began by reducing the primary spatial polygons data frame—effectively, the map of all colonies—to a subset of colonies that were capable of growth. This subset excluded all colonies that were completely enclosed by neighboring colonies as well as those whose colony sizes were insufficient to warrant territory expansion beyond their current extents. To determine whether a colony was large enough to grow its territory, we calculated the expected number of workers for the current territory size based on the density of workers per area in mature colonies (1 worker per 6.4 cm2, Tschinkel et al. 1995). If a colony’s size (calculated in *Step 2: Colony growth*) exceeded that expected from its territory size, then we included it among those slated for territory expansion.

For each territory to be expanded, we then used the *gBuffer* function in the *rgeos* package (Bivand & Rundel 2015) to draw a buffer around the territory. The width of the buffer was determined by the territory size of the colony, such that larger territories were assigned larger buffers:

buffer width = (colony area)0.5 \* 0.2

After establishing a buffer area around each colony territory, we used the *gDifference* function in the *rgeos* package (Bivand & Rundel 2015) to subtract from the buffers all areas occupied by existing colonies and areas beyond the arena boundaries. The remaining polygons outlined the areas into which territory growth was possible, and were added to the colony’s current territory. In many cases, however, the potential growth areas of different colonies overlapped. When this occurred we overlaid a 4 x 4 grid on the overlapping area, dividing it into subpolygons. We then assigned equal numbers of grid cells to the two parent territories. We did this in a manner that ensured that grid cells were not separated from the parent territories to which they were assigned. Overlapping potential growth areas were thus divided between two parent colonies roughly equally. This means of allocating space applied only to pairwise overlaps. In cases where potential growth polygons from three or more colonies overlapped, we first divvied up the overlap associated with the two oldest colonies from the group and then assigned the remaining area to the other parent colonies. In cases where large colony territories grew to completely surround smaller ones, the subsumed colony was deleted and the larger one allowed to expand into the vacated area, reflecting the competitive dominance of large colonies and their intolerance of smaller colonies within their borders (Tschinkel 2013).

Once all territory sizes were adjusted, we again calculated the expected colony size based on territory size (1 worker per 6.4 cm2, Tschinkel et al. 1995), and compared this value with the current colony size (see *Step 2: Colony growth*). The lesser of the two values was retained as the colony size for the current time step. In this way colony and territory growth interacted in a mutual feedback, such that potential colony growth at each time step determined the potential for territory expansion, and realized territory expansion allowed or limited realized colony growth. This feedback captures the situation in the field, in which the number of workers in a colony determines its competitive ability, but a colony’s territory size determines the resources available for the production of workers (Tschinkel 2013). Colony territories do not shrink when the number of workers declines due to seasonal fluctuations (Tschinkel et al. 1995). Territory sizes in our model therefore remained static during seasonal worker declines or following the death of queens (see *Step 2: Colony growth*).

Simultaneously expanding individual territories in a manner that fills available space but does not allow overlap was difficult, largely due to the frequent generation of topographies that were invalid or incompatible with the spatial functions we employed. Invalid topographies often included self-intersecting polygons or complex polygons that closed into lines upon territory expansion. To avoid some of these errors, we rounded polygon coordinates to the nearest millimeter. We alleviated the vast majority of errors that still occurred by using the *clgeo\_Clean* function from the *cleangeo* package (Blondel 2015), which corrected problematic polygons, with negligible changes to their areas and outlines. Rare topology errors, however, still arose that could not be handled. In these instances we determined which of the polygons in the spatial polygons object let to the invalid topography and deleted it. These errors occurred only up to 10 times for each 300-month simulation involving over 10,000 colonies, and we do not think they compromised our results. When the previous measures failed to avoid invalid topographies, we implemented a routine that essentially went back in time in the simulation to January of the preceding year (12 to 23 months before the error was encountered). When this happened, all model parameters reverted to a state stored in memory corresponding to that particular January. The simulation then proceeded forward, and due to the stochasticity in the model was unlikely to encounter the same error. The end result was a model structure that could complete a 300-month simulation about 95% of the time.

*Step 4: Reproduction and dispersal*

Once fire ant colonies grow sufficiently large, they begin producing queens to disperse and reproduce. In our model, colonies started to produce queens after growing to 30,000 workers in size (Markin et al. 1973, Vargo 1988). For each colony for each year, we determined queen production based on its size in January, which is an indicator of the energy reserves available for reproduction (Tschinkel 1993). Colonies with fewer than 50,000 workers in January produced enough queens to weigh 16% as much as the colony’s combined worker biomass, whereas larger colonies produced enough to equal 35% of worker biomass (Tschinkel 1993). Determining worker biomass from the number of workers is not straightforward, as larger colonies produce larger individual workers. We thus calculated total worker biomass nonlinearly:

worker biomass = 0.086 \* *P*1.178

where *worker biomass* is dry mass measured in milligrams and *P* equals the number of workers in the colony (derived from Figure 23 in Tschinkel 1993).

To translate total queen biomass into individual queens, we first determined the relative investment in claustral versus parasitic queens. We did this using a variable, *ptype*, which could range from ~0 to 1 and represented the proportion of queen biomass invested in claustral queens. The value of *ptype* was assigned to the initial colonies in each simulation, was inherited by daughter colonies thereafter, and varied across simulations (see *Experimental design*). We divided the total mass of each queen type by average queen mass to determine the total number of queens to produce that year. For this step we assumed an average dry mass of 4.7 mg for parasitic queens and 7.2 mg for claustral queens (Helms & Godfrey 2016). Finally, to simulate the near total mortality that occurs during mating and early colony founding, we randomly deleted 95% of the queens of both types produced by each colony. Mortality among dispersing fire ant queens is known to be high (estimated at over 99%, Whitcomb et al. 1973, Tschinkel 1992) but is difficult to measure. Our value of 95% is therefore just an estimate. The simulation results were not sensitive to this random queen mortality, however, as the arenas were nearly fully occupied by territories, and competition for space appeared to be the dominant driver of colony growth (see *Results*). The remaining queens from all colonies were added to a data frame that recorded their type and colony of origin.

Although annual queen production was determined in January, queen dispersal took place over several months throughout the year. For parasitic queens, half the queens dispersed in February and half in March (Morrill 1974, Tschinkel 1996). Claustral queens dispersed in the spring and summer—20% in April, 20% in May, 30% in June, 20% in July, and 10% in August (Morrill 1974). Queens dispersed away from their parent colony according to random draws of direction and distance. Direction was drawn from a uniform distribution of 0 to 360 degrees. For claustral queens distance was drawn from a gamma distribution with a mean of 20 meters and a standard deviation of 2 meters. For parasitic queens we used a gamma distribution with a higher mean and standard deviation (30 ±3 meters), to reflect the more favorable flight morphology that results from their reduced weight (Helms & Kaspari 2014, 2015, Helms & Godfrey 2016). Fire ant queens in the field routinely disperse several hundred meters and occasionally several kilometers (Tschinkel 2013, Helms et al. 2016a, b). Our dispersal distances are thus not realistic. Attempts to use more realistic dispersal distances resulted in extremely large numbers of colonies that caused simulations to progress slowly and eventually crash. Based on these trials, however, simulations with long dispersal distances appeared to have the same dynamics as those with short distances, with the exception that farther dispersal causes populations to expand their ranges more rapidly. Queens that dispersed across the lower side of the arena, the only bounded edge, were considered dead and we deleted them. Those that flew across the right or left edges of the arena were repositioned within the arena but on the opposite side, as if the left-right dimension was continuous and circular (*i.e.*, a cylinder). There were no constraints on upward dispersal.

Survival and successful colony founding depended on where a queen landed. Claustral queens that landed within an area occupied by any existing colony were killed. Those that landed on unoccupied space, however, were transformed in the next time step into newly established colonies, each with 40 workers and a territory of 0.1 m2 (see *Step 2: Colony growth*, Figure 1b). Parasitic queens, on the other hand, survived only if they landed within the territory of an orphaned colony (see *Step 1: Colony mortality*, Figure 1c) and were killed if they landed in unoccupied space or the territory of a colony whose queen was alive. If two or more claustral queens landed in unoccupied space close enough for their initial territories to overlap, or if multiple parasitic queens landed within the same orphaned colony’s territory, a single winning queen was chosen at random and the remaining queens killed. Orphaned colonies that received a parasitic queen retained their current colony and territory size, were no longer considered to be orphaned, and began to grow again (see *Step 2: Colony growth*). They were, however, assigned new parameters for parent lineage, age, and *ptype* matching those of the new queen.

*Step 5: Advancing to the next time step*

After any newly established colonies were added to the spatial polygons data frame, we performed error checking steps to ensure that the topology of the new set of polygons was acceptable (see *Step 3: Territory growth*). The updated data frame was then saved, and we advanced counters that kept track of the time step and calendar month. The entire process was then repeated for the next time step.