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AN AGENT-BASED SIMULATION MODEL OF SPONGE:ALGAE SYMBIOTIC RELATIONSHIPS

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ABSTRACT

One of the most important ecological interactions that occurs in shallow tropical habitats worldwide involves trophic (feeding) interactions between symbiotic dinoflagellate algae and a variety of invertebrate and protistan hosts, such as sponges and coral. The algal symbionts, known as *Symbiodinium*, reside within the host cells, and have long been recognized to be of vital energetic importance to the host. Unfortunately, the dynamics of the associations (e.g., symbiont population growth behavior, loss of symbionts from the host, competition among different symbiont types, host responses to symbionts of different quality) are poorly understood. This paper presents an agent-based simulation model for studying the symbiotic relationship between algal symbionts and host sponges. Initial results demonstrate realistic behavior by the model and suggest important future research directions, coordinating model extensions with experiments to be performed in tropical habitat field work.

1 INTRODUCTION

Coral reefs are among the most biologically diverse, and economically important, ecosystems on the planet despite covering only 0.2% of the ocean floor (Spalding et al. 2001). The entire coral reef ecosystem is supported by mutualistic symbioses that occur between animal hosts (e.g., corals) and their algal symbionts known as *Symbiodinium*. The symbionts live in membrane-bound compartments inside host cells (Davy et al. 2012). From this intracellular position, the algae nourish their hosts through the transfer of photosynthetically-derived sugars and other materials (Stambler 2011, Davy et al. 2012). These symbionts are efficient photosynthesizers, and can provide a large portion of the energy that the coral:symbiont combination requires to grow and reproduce. Environmental stressors like elevated sea surface temperatures caused by global climate change can cause the relationship between many coral hosts and *Symbiodinium* to break down. This phenomenon, known as coral bleaching, is one of the factors that has led to world-wide declines in coral reef habitats. Approximately 19% of the world's reefs have already been lost, and an additional 20% of existing reefs could be lost in the next 20-40 years (Wilkinson 2008).

Corals are not the only hosts that harbor *Symbiodinium* symbionts. Other cnidarian and non-cnidarian hosts harbor intracellular populations of *Symbiodinium* (Pochon et al. 2010, Hill et al. 2011). These symbioses offer the opportunity to find commonalities in the pathways that symbionts use to gain entry into host cells. Several sponge species, notably the bioeroding clionaids, support sizeable *Symbiodinium* populations within their tissues. Clionaids provide a unique opportunity to explore aspects of host biology that permit invasion and establishment of *Symbiodinium* populations. Unlike cnidarians, *Symbiodinium* found in sponges are not restricted to a particular layer of endodermal tissue, and can occur deep in the sponge body (Hill and Hill 2012). Furthermore, *Symbiodinium*-bearing sponges can bleach in a manner

that is distinct from coral bleaching (Hill and Wilcox 1998), the hosts rely on energetic contributions from the algae (Weisz et al. 2010), and the symbionts induce intriguing patterns of host gene expression (Riesgo et al. 2014). Finally, the filter-feeding characteristics of sponges create a high probability that these potential hosts will come into contact with algae suspended in the water column (Scalera-Liaci et al. 1999). Accordingly, our focus in this paper is on sponges as the model host.

Despite the importance of the host:*Symbiodinium* symbiosis to the entire coral reef ecosystem, there is still much to learn about the dynamics of algal populations within the host under benign and stressful environmental conditions (Davy et al. 2012). The density of algae fluctuates through time, but the factors that shape those patterns are poorly understood. Furthermore, most host:*Symbiodinium* associations are highly specific with significant fidelity between partners — i.e., the type of algae residing in a host's cells are typically specific to that species of host and vice versa (Thornhill et al. 2009). The conditions that allow this type of partner specificity to evolve are also poorly understood. While the dynamics of establishing the partnership from one generation to the next are complex, the route of symbiont entry into many hosts is via phagocytosis (ingestion). Once a symbiont cell is captured, it must navigate the cellular machinery of its host to avoid digestion.

A recent hypothesis proposes that phagocytosed symbionts avoid digestion by mimicking digesting prey through the transfer of photosynthetically-derived sugars to the host cell (Hill and Hill 2012). The cost of transferring photosynthate may reduce the rate of cell division, which would limit symbiont population growth (Hill 2014). Careful testing of these and other hypotheses is needed to explain observed patterns of symbiont population growth and decline. However, the field experiments required to fully test these hypotheses are prohibitively complicated and expensive. A detailed computational model simulating symbiont population dynamics within a host offers the potential to run controlled experiments designed to test specific predictions of hypotheses, and will help to identify the most important parameters of interest before embarking on empirical tests.

Several general models have been constructed to explain the evolution of mutualistic interactions among partners (e.g., see Sachs et al. 2004), most often as compartmental (population dynamics) models (e.g., Holland et al. 2002). Specific models have been developed to describe the symbiotic relationship between *Symbiodinium* and their hosts (e.g., Hallock 1981, Stoecker 1998). For example, Day et al. (2008) modeled the evolution of bleaching resistance in corals, and Muller et al. (2009) used dynamic energy budgets to explore the effects of host physiology on symbiont density.

One primary drawback of compartmental models is the frequent assumption that each compartment (category) consists of a set of homogeneous individuals, and incorporating complex low-level dynamics is limited in scope. Because of the ability to easily model heterogeneous populations in detail, agent-based models apply well in this context. Indeed, a recent call (Helbing and Balietti 2011) indicates that these models provide natural heterogeneity and are well suited for detailed hypothesis testing. Although agent-based models have a robust history in ecological research, the majority of work in coral reef environments has focused on ecosystem- or community-level perspectives (e.g., Yniguez et al. 2008, Canal-Vergés et al. 2014) but not on understanding intracellular mutualisms.

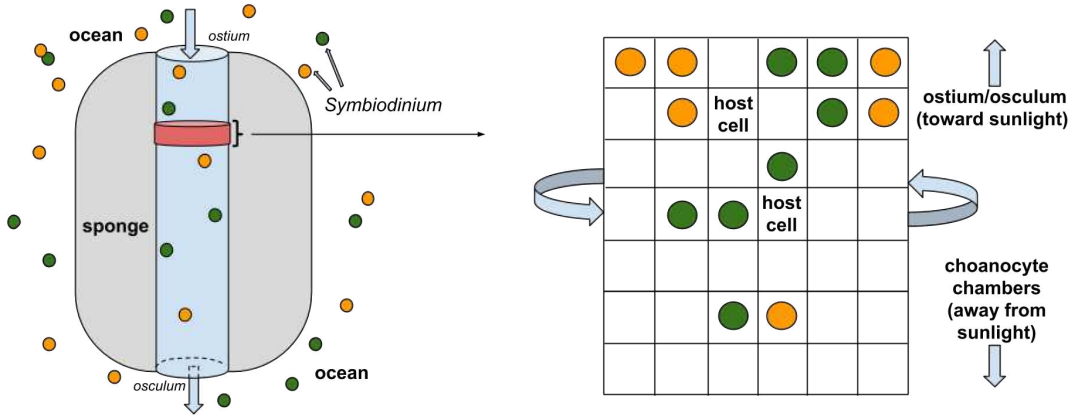
The contribution of our work lies in the introduction of a computational model that, as realistically as possible, simulates the complex host:*Symbiodinium* relationships present on coral reefs. This paper describes an agent-based model that simulates interactions between a sponge host, its *Symbiodinium* symbionts, and the environment that these organisms reside in. We provide preliminary results demonstrating the ability of the model to capture the complex dynamics associated with host:symbiont interactions. The model offers the opportunity to explore nuanced aspects of host:symbiont interaction, which will lead to a suite of predictions that can be tested using field and lab experiments. Our approach allows for exploration of factors that may contribute to the establishment and long-term maintenance of intracellular symbiont populations, and may identify novel strategies that symbionts employ to secure their position within a host. This is a promising approach to increase the rate of discovery of the most important processes that regulate host:symbiont interactions on coral reefs.

The remainder of this paper is organized as follows. Section 2 provides a detailed description of the sponge environment and the various states of symbionts in that environment. Our agent-based simulation model is discussed in Section 3. Section 4 discusses experiments and results using our model, and Section 5 provides conclusions and future directions.

2 SPONGE ENVIRONMENT AND SYMBIONT STATES

The dynamics of the relationship between symbionts and sponges (as well as competition between and among different clades of symbionts within a sponge) are not well understood, but many of the processes that govern the symbiont's habitation within the sponge, of symbiont cell division, and of symbiont death are known (Davy et al. 2012, Hill 2014).

As discussed in Section 1, a symbiont resides in a membrane-bound compartment within one of the sponge's host cells (Davy et al. 2012). This process of residence occurs as the sponge pumps water from the surrounding ocean through a canal in the sponge. As depicted in Figure 1a, symbionts in the ocean may be pulled into the *pool* of water in this canal, and occasionally come into contact with cells on the lining of the canal. (Note that symbionts may come to reside within host cells farther inside the sponge body, but this is beyond the scope of our model. We consider only the lining of the canal.)



(a) (b)

Figure 1: (a) Water from the ocean is pumped by the sponge through a canal, in which symbionts in the water may come into contact with, and potentially inhabit, host cells on the exterior of the canal. (b) Two-dimensional grid model of a slice of that sponge canal.

For our model, Figure 2 depicts the various states that a symbiont may have during its life cycle relative to its contact with the sponge. These states are described below.

- A symbiont in the pool within the sponge canal may come into contact with a host cell (I).
- Provided there is sufficient affinity between the host cell and contacting symbiont, the symbiont takes up residence within the cell through a process known as *phagocytosis* (IIa). Otherwise, the symbiont escapes back into the pool (IIb).
- Once in residence within the host cell (III), the symbiont continues to photosynthesize, producing energy (*photosynthate*) that can be used by the symbiont and by the host cell (Hill and Hill 2012). Provided the photosynthate produced is sufficient to sustain the symbiont and also meet the energy demands of the host cell, the symbiont will continue to inhabit the host cell. Otherwise, the symbiont may be digested by the host cell (IVa) or may escape prior to digestion occurring (IVb).

- A symbiont in residence within the host cell will continue its natural process of cell division (*mitosis*), attempting to produce another symbiont (V). (Note that mitosis may occur outside the context of host cell habitation, but that is beyond the scope of our work.)
  - Because mitosis requires an energetic cost of the symbiont, during mitosis there may be insufficient photosynthate to meet the energy demands of the host cell, in which case the dividing symbiont may either be digested (Va) or may escape into the pool before division completes (Vb).
  - Provided the dividing symbiont can produce enough photosynthate to complete the division while still meeting host cell demand, a new symbiont is produced. If there is no unoccupied adjacent host cell available for the symbiont, either the original or new symbiont will be evicted into the pool (Vc). If there is an unoccupied adjacent host cell, the new symbiont is phagocytosed by that cell (Vd), at which point the new symbiont begins intracellular residency. (Because the new symbiont is an exact copy of the original symbiont, there should be sufficient affinity between the new symbiont and the adjacent host cell.)
- Finally, at some point during its residence a symbiont simply may exit the host cell (*denouement*) returning back into the pool (VI). This denouement is not a result of insufficient photosynthate production, and so is distinct from the pre-digestion escape discussed above.

Except for the process of initial residence (which may occur as a result of arriving from the pool or via mitosis), these same states hold for all symbionts in the system.

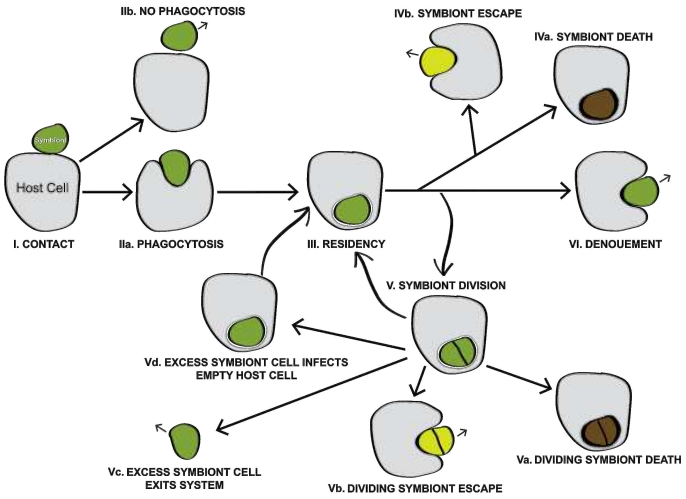
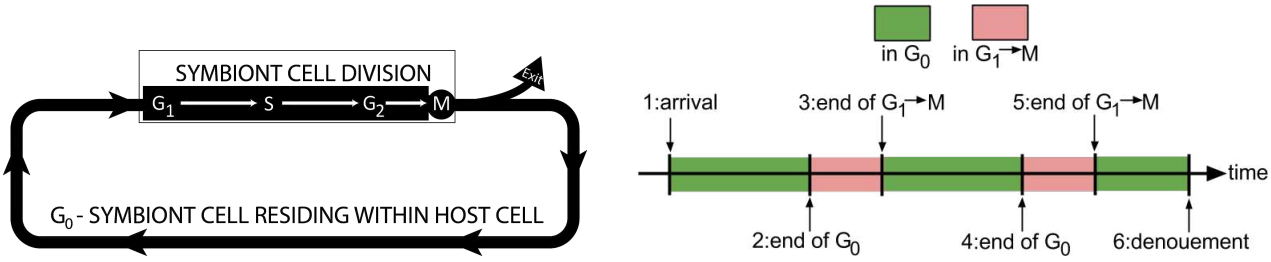


Figure 2: State diagram for algal symbionts in the sponge environment.

We now provide more details on the steps of mitosis discussed above. Once a symbiont is in residence inside a host cell, the symbiont repeats a process in which it attempts to divide. This process can be represented as a "clock", during which the symbiont initially caches photosynthate in preparation for division, followed by the division process itself. As shown in Figure 3a, the entire process consists of five phases: G_0, G_1, S, G_2, and M. During the G_0 phase, the symbiont resides within the host cell, producing sufficient photosynthate to satisfy the host cell demand while caching the surplus. Once the symbiont enters the four division phases (G_1, S, G_2, M), the symbiont is then committed to the division process. If the symbiont cannot successfully complete the division (because the demand for energy from the host cell plus the energetic cost of the division is too high), the dividing symbiont may either be digested or may escape, as discussed above. If the symbiont can complete the division, either of the two resulting symbionts must occupy an adjacent host cell or, if none is available, be evicted into the pool. Upon successful division, the entire process (G_0, G_1, S, G_2, M) repeats for that symbiont, and the process starts for any progeny symbiont.



(a) (b)

Figure 3: (a) The cell cycle, consisting of five phases: G_0, G_1, S, G_2, and M. Once phase G_1 begins, the symbiont is committed to the division process until phase M completes. As indicated, one of the two resulting cells must find a new host cell. (b) Example timeline of events for a symbiont.

3 AGENT-BASED MODEL OF THE SPONGE / SYMBIONT ENVIRONMENT

We use an agent-based model to simulate the interactions of symbionts with their sponge environment as well as competition among symbionts, particularly symbionts of different clades. The goal of agent-based modeling in general is to realize global-scale behavior patterns that emerge from the definition of local-scale rules. Agent-based modeling consists of a collection of agents (autonomous, heterogeneous individuals), an environment in which the agents reside, and a collection of rules that govern how the agents interact with one another and with the environment.

The environment in our model is the sponge, consisting of a collection of host cells for symbiont habitation. As depicted in Figure 1a, symbionts being pumped through the sponge from the ocean may come into contact with host cells on the lining of the sponge canal. (Recall from Section 2 that symbionts residing in host cells farther inside the sponge body are beyond the scope of our model.) To avoid the need to model water flow effects, we model the environment as a "slice" of the sponge canal, represented by a 2-D grid of host cells as shown in Figure 1b. The 2-D grid wraps horizontally consistent with the canal; the upper portion of the grid is presumed closer to the ostium or osculum (closer to sunlight) while the lower portion is presumed closer to the choanocyte chambers, which via flagella generate water flow, in the center of the sponge (away from sunlight). In this way, symbionts closer to sunlight (near the top of the grid) will produce photosynthate at a higher rate than symbionts closer to the choanocyte chambers (near the bottom of the grid). No more than one symbiont may occupy a host cell in the grid at any time. Each host cell has a particular photosynthate demand of any symbiont residing inside.

An agent in our model represents a symbiont: each symbiont agent has a set of characteristics (data) uniquely populated per symbiont, as well as set of behaviors (methods) consistent with the actions of symbionts discussed in Section 2. For a symbiont, the set of characteristics includes:

- cell: the sponge host cell currently being occupied by the symbiont;
- clade: the clade (symbiont group) to which this symbiont belongs;
- mitotic class: how frequently the symbiont attempts division;
- production rate: the number of units of photosynthate produced by this symbiont per unit time;
- photosynthate surplus: the number of units of photosynthate cached by this symbiont (i.e., produced but not lost to host cell demand or to energetic cost of mitosis).

As discussed above, the rate of photosynthetic production is a function of symbiont location in the environment. For this work, we presume that production rate decreases linearly from a maximum rate P for symbionts occupying the top row of the host cell grid to a minimum rate P/k for symbionts occupying the bottom row, where k is a parameter whose value is defined at run-time.

We use an event-oriented world view to govern the time evolution of our simulation model. Accordingly, the set of event types for the discrete-event simulation model corresponds to the set of behaviors for a symbiont, and includes the following:

- arrival: When a symbiont arrives, it is assigned a clade at random. Provided there is sufficient affinity (associated with the clade) between the symbiont and host cells, an unoccupied host cell is selected at random and the symbiont inhabits that cell. The symbiont immediately enters the G_0 phase (see the example in Figure 3b). If the symbiont will survive in the host cell until the end of G_0 (i.e., produced and cached photosynthate is sufficient to satisfy host cell demand), an end-of-G_0 event is scheduled for the symbiont; otherwise, a digestion event is scheduled at the time photosynthate cache reaches zero, or via weighted coin flip an escape event is scheduled prior to digestion. (Because the times for affinity-to-residency, for digestion, and for escape are each likely negligible in comparison to reproduction times, we model these times to have length zero.)
- end G_0: The symbiont immediately enters the $G_1 \rightarrow M$ phase (see Figure 3b). If the symbiont will survive in the host cell until the end of $G_1 \rightarrow M$ (i.e., produced and cached photosynthate is sufficient to satisfy host cell demand and energetic cost of mitosis), an end-of-$G_1 \rightarrow M$ event is scheduled for the symbiont; otherwise, a digestion event is scheduled at the time photosynthate cache reaches zero, or via weighted coin flip an escape event is scheduled prior to digestion.
- end $G_1 \rightarrow M$: This successful mitosis results in an additional symbiont being created. The new symbiont is placed at random into an unoccupied host cell in the Moore neighborhood around the current cell. If there is no unoccupied cell, via weighted coin flip one of the two symbionts is evicted into the pool while the other maintains residence in the current cell. (Note: In the uppermost and lowermost rows of the 2-D grid, there may be unoccupied cells just outside the range of our grid that the new symbiont could inhabit. In these cases, within the Moore neighborhood we model the number of open cells in the three cells outside our grid according to the proportion of open cells in the five cells inside our grid. Accordingly, the new symbiont may "occupy" one of the three adjacent cells outside our grid, corresponding to the symbiont leaving our system.)
- digestion: The symbiont is digested immediately, a result of unsuccessfully completing a G_0 or a $G_1 \rightarrow M$ phase, and is therefore no longer part of the system.
- escape: The symbiont leaves the system immediately, a result of unsuccessfully completing a G_0 or a $G_1 \rightarrow M$ phase, avoiding digestion and returning to the pool.
- denouement: The symbiont leaves the system immediately, after a sequence of successful mitoses, returning to the pool.

We specifically note that we are implementing the cell cycle from Figure 3a as only two distinct events: G_0 and $G_1 \rightarrow M$. This is reasonable because, as discussed earlier, once the symbiont enters G_1, it is committed to the entire division process.

Figure 3b depicts an example timeline of six events for a particular symbiont. In this example, the symbiont arrives and inhabits a host cell as a result of sufficient affinity with that cell (event 1). While in G_0 (e.g., between events 1 and 2), the symbiont is producing photosynthate, caching any that is not lost to host cell demand. While in $G_1 \rightarrow M$ (e.g., between events 2 and 3), the symbiont is producing photosynthate, caching any that is not lost to host cell demand nor to energetic cost of mitosis. This example symbiont successfully finishes two complete cell cycles (events 2–5), with a new symbiont resulting from each of events 3 and 5. In this example, before entering a third $G_1 \rightarrow M$ phase, the symbiont leaves the system, returning to the pool (event 6).

Finally, our simulation model includes a collection of parameters, with values defined at run-time, that allow for careful benchmarking and experimentation. These parameters include: (a) size of 2-D sponge grid; (b) rate of photosynthate demand by host cells (min,max); (c) number of symbiont clades; (d) proportion per clade of symbionts in the ocean; (e) affinity per clade with host cells; (f) maximum photosynthetic production rate per clade; (g) maximum expected residence time per clade; (h) average length of G_0 (per

clade); (i) average length of $G_1 \rightarrow M$ (per clade); (j) rate of energetic cost of mitosis; (k) G_0 escape probability (vs. digestion); (l) $G_1 \rightarrow M$ escape probability (vs. digestion); (m) initial photosynthate cache on arrival (min, max); (n) reduction factor k of minimum photosynthetic production rate in bottom row of 2-D grid; (o) maximum simulated time; and (p) average time between arrivals.

4 RESULTS

The goal of the results presented here are to qualitatively discuss and assess the demonstrated behavior of our model, rather than to provide precise quantitative results. Precise quantitative validation of the model requires extensive field work, and is appropriate for an audience with research expertise in the dynamics of sponge:*Symbiodinium* interactions. Accordingly, such quantitative analysis is beyond the scope of this paper and is deferred for future work. Instead, we assess the accuracy of our model by qualitatively assessing demonstrated behavior, relying on the expertise and insight of the biologist coauthors who have extensive experience in sponge:*Symbiodinium* research.

Our agent-based model was implemented using Python, leveraging object-oriented capabilities for implementing the agents, the environment, and the event-oriented simulation engine. For all results to follow, we conducted experiments by varying the values of select parameters relative to baseline values for those parameters. Some of these baseline values were chosen consistent with values for *Symbiodinium* available in the biological literature. Other baseline values are not established in the literature, and are instead chosen based on the observations of the biologist coauthors. The baseline parameter values for our experimentation are given in Table 1.

Table 1: Baseline parameter values for our model.

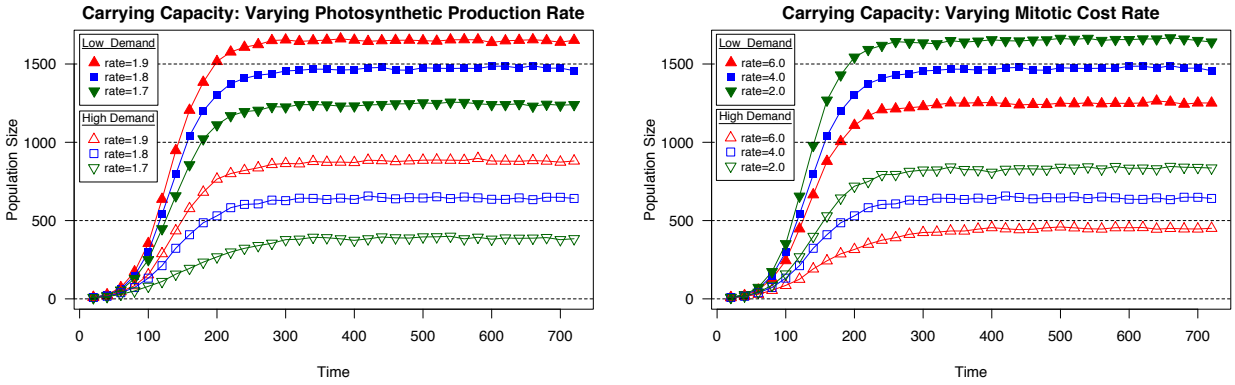
Host cell grid size	50×50
Simulated time	730 (days)
Average time between arrivals	1.0 (days)
Photosynthetic production rate	1.8 (units)
Mitotic cost rate	4.0 (units)
Host cell demand range (low)	(1.0,1.4) (units)
Host cell demand range (high)	(1.3,1.7) (units)

Maximum expected residence time	58 ± 1 (days)
Expected G_0 length	13 ± 1 (days)
Expected $G_1 \rightarrow M$ length	1 ± 0.1 (days)
Prob. of symbiont affinity	0.5
Prob. of G_0 escape (vs. digestion)	0.5
Prob. of $G_1 \rightarrow M$ escape (vs. digestion)	0.5
Prob. dividing symbiont evicted (no vacancy)	0.5
Production-rate linear decrease factor k	2 (see §3)

We also note that the unit of time in our simulation is one calendar day, and that inter-arrival times are generated using an exponential distribution. For symbionts arriving from the ocean (not via division), their initial photosynthate surplus is chosen at random from the range (D, $10D$), where D is the maximum host cell demand given in the table above. (This cache-on-arrival is consistent with realistic evolutionary strategies, and gives symbionts who are unfortunate enough to land in a cell farther from the sun the opportunity to reside for at least a short while.)

Of particular interest to biologists is the carrying capacity of the sponge environment: the number of symbionts residing in the sponge's host cells across time. The factors that distinguish a situation where symbionts are thriving in a healthy host environment versus exiting from a stressed host environment are poorly understood. To that end, we are interested in investigating how carrying capacity of the symbiont population responds when we vary particular parameter values. For the results that follow, we limit the population to one symbiont clade (group), and presume that the sponge starts initially empty (mimicking a bleached starting point).

Figure 4a depicts the carrying capacity as a function of varying symbiont photosynthetic production rate. The uppermost three curves correspond to an environment of lower host cell demand (see Table 1) and the lowermost three curves to an environment of higher host cell demand. We note that simply changing cellular energetic demand by the host causes a dramatic shift in the population size of symbionts (uppermost vs. lowermost curves). This suggests that host cellular physiology alone might explain some of the patterns in symbiont density seen on coral reefs and in other phototroph:heterotroph symbioses. Furthermore,



(a) (b)

Figure 4: (a) Sponge environment carrying capacity as a function of varying the symbiont photosynthetic production rate. (b) Carrying capacity as a function of varying the symbiont mitotic cost rate.

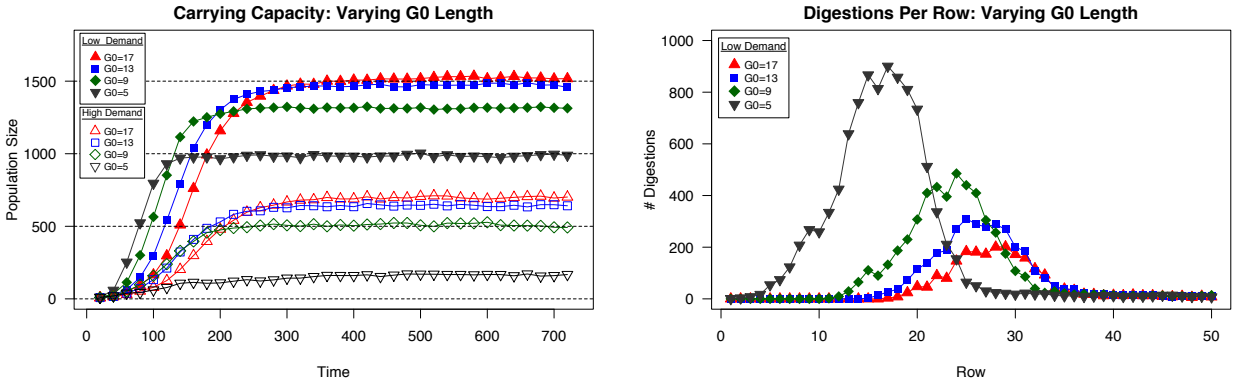
we observe that small changes (5-6%) in photosynthetic production rate can lead to substantial increases in carrying capacity. Indeed, based on these results, we observe increases of roughly 20% in symbiont population size within each of the low- and high-demand host scenarios.

Similarly, Figure 4b depicts the carrying capacity as a function of varying cost rate of mitosis for the symbionts. Again, the figure is presented in scenarios of a low- and high-demand host. Host cellular physiology seems to be exceptionally important in shaping symbiont population carrying capacity when only the cost of symbiont mitosis is considered. The gap between symbiont population sizes in high versus low cell-demand scenarios is significant, and suggests a two-fold increase in the cost of residing in a high-demand host cell environment. If the host cell energy expectancy is high (i.e., residency is expensive), the danger of symbiont cell division is clear, as significant withdrawals from photosynthetic caches of symbionts corresponds to a reduced population size. This is supported by the fact that we observed more symbiont digestions and escapes under high cell-demand than under low cell-demand.

The rate increases in Figure 4 generate results that match expectations of symbiont population behavior. As symbionts are able to produce more photosynthate on average (e.g., nearer the sun), more symbionts will be able to reside within the sponge. Similarly, a lower cost for mitosis will result in more successful divisions, thereby increasing the resulting population size of symbionts. We also note that the rates of growth in symbiont population vary most significantly in the high cell-demand scenario (e.g., the rates of growth of the bottommost three curves in Figure 4a). This observation warrants a more detailed investigation from the biological perspective, and suggests that, as symbionts escape or are digested more rapidly, it takes longer to reach a phase of maximal population growth.

Figure 5a depicts the carrying capacity as a function of varying the expected length of G_0 for symbiont cell division, both in low- and high-demand host scenarios. We note that there are marked differences in rates of growth of the carrying capacity curves. A faster cell cycle (i.e., smaller G_0 length) corresponds to more divisions and therefore to a faster rate of occupancy. We note three biologically interesting trends from these results. First, the rate of cell division influences overall carrying capacity. Second, the effect of rates of cell division become magnified (i.e., they demonstrate a non-linear influence) on the shape of the population growth curve and the final carrying capacity. Third, different rates of cell division lead to different times required to achieve equilibrium in the carrying capacity.

The results described above are supported by further investigation into events occurring in the model. Figure 5b depicts the number of digestions per row of the host cell environment for different G_0 lengths. (Though omitted for brevity, a figure depicting the number of escapes, i.e., to avoid digestion, per row is qualitatively similar.) In general, a faster cell cycle (lower value for G_0 length) corresponds to more digestions and escapes. We hypothesize that this is a result of symbionts making "energetic mistakes",



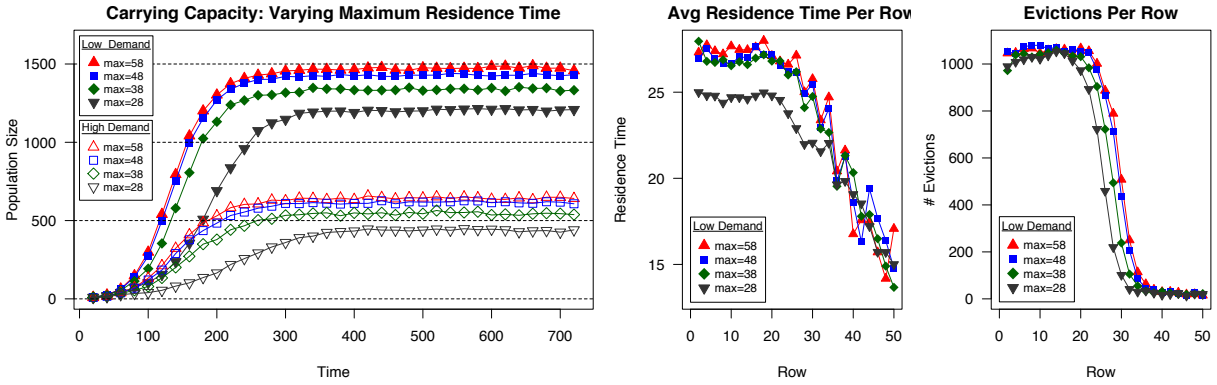
(a) (b)

Figure 5: (a) Sponge carrying capacity as a function of varying the symbiont expected G_0 length under low and high cell demand. (b) Digestions per row for varying G_0 length under low cell demand.

i.e., that attempting division more frequently results in more opportunities to divide when the cached photosynthate is insufficient to support the division to completion (thus triggering digestions or escape). It is also interesting to note that the majority of digestions and escapes occur closer to the center of the sponge model grid. This is to be expected, as symbionts residing at the top of the grid will have highest photosynthetic production rate, and are therefore less likely to be digested or need to escape. As photosynthetic production rate decreases with increasing row, the number of digestions and escapes should increase (middle rows of the grid), as shown. However, eventually that decreasing production rate will result in a region (lower rows of the grid) where habitation by symbionts is less likely. With fewer symbionts in residence in that region, the number of digestions and escapes there will be correspondingly low.

Figure 6a depicts the carrying capacity as a function of varying the maximum residence time for symbionts, both in low- and high-demand host scenarios. Again it is evident that the host cell demand has a significant impact on carrying capacity. We note that, under this collection of parameter values, varying the maximum residence time does not have as dramatic an effect overall as did varying the other parameters above. Indeed, successive increases to the maximum residence time result in successively smaller increases in the carrying capacity. This results primarily from the fact that, even with a large value for expected maximum residence time, very few symbionts ever reach that corresponding denouement event. Figure 6b depicts the average symbiont residence time per row and shows that even in the upper rows of the sponge (where symbionts could be expected to reside longest), the average residence time is much less than the maximum. This can be explained by a high number of mitotic evictions in the upper rows, as shown in Figure 6c. Recall that when successful mitosis occurs, if there is no open cell for the new symbiont then one of the two resulting symbionts will be evicted into the pool. Because the concentration of symbionts (and correspondingly the number of attempted divisions) is higher in the upper rows, and because the choice of symbiont to be evicted is by fair coin flip (see Table 1), few of the symbionts will persist in residence until denouement.

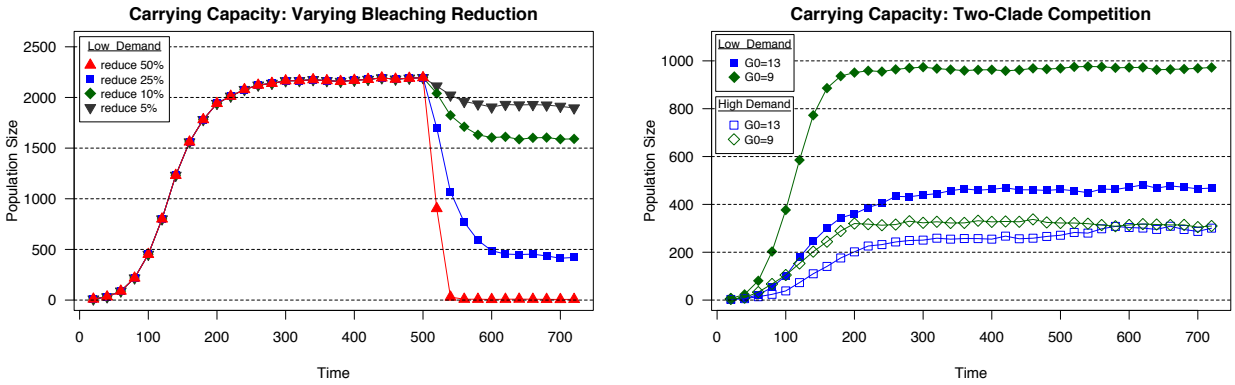
One important test of this model is to determine whether we are able to mimic bleaching events that are expected when sea surface temperatures approach or exceed 32°C (a global warming scenario). Figure 7a depicts the results of simulating a warming event that occurs at day 500 by decreasing the photosynthetic production rate of symbionts by a given percentage. (Note that for this particular experiment only, we used a production-rate linear decrease factor of $k = 1.5$, which has the effect of allowing more symbionts to reside lower in the grid, thereby increasing the expected carrying capacity.) The consequence of this drop in photosynthesis matches our expectations given that, particularly with a large percentage decrease in production rate, it results in drastic changes in symbiont population carrying capacity. This demonstrates the ability of this model to predict host:symbiont breakdown as a result of declines in symbiont performance.



(a) (b) (c)

Figure 6: Under varying maximum expected residence time: (a) sponge environment carrying capacity under low and high cell demand; (b) observation-averaged residence time per row; (c) mitotic evictions per row. The middle and right plots are under low cell demand only.

As shown in Figure 7b, we also conducted a competition experiment where two different clades of symbionts infect a single host. The two clades were identical with the exception of expected length of G_0 for mitosis. In the low cell-demand environment, faster rates of cell division (lower G_0) led to higher symbiont carrying capacity, and a faster rate to achieve that population size. The low cell-demand environment is a less stressful environment for the symbiont, which allows a fast-growing clade (lower G_0) to rapidly propagate into empty cells since few resources are diverted to satisfy the demands of the host. The success of symbiont type 1 (lower G_0) is caused by its ability to reduce the number of host cells available for symbiont type 2 to infect. Under the more stressful high cell-demand environment, symbiont type 1 had a faster rate of growth, but across time neither clade was able to dominate the other. This type of demanding environment causes all symbionts to divert resources to satisfy the host, depressing the growth rates for all symbionts and therefore giving the slower-growing clade a competitive chance. These results demonstrate the power and utility of this modeling approach to simulate realistic scenarios of cladal competition, and our model opens many avenues for empirical testing.



(a) (b)

Figure 7: (a) Sponge environment carrying capacity with one clade in the presence of a bleaching event at time 500 under low cell demand. (a) Sponge environment carrying capacity with two clades differing only in G_0 length under low and high cell demand.

5 CONCLUSIONS AND FUTURE WORK

Coral reef ecosystems are facing worldwide degradation, and if current trends continue, a significant percent of the world's coral reefs could be destroyed over the next 30 years. Understanding the dynamics of the intracellular symbiosis between hosts and algal partners in coral reefs is critical for slowing these trends. To that end, we have presented a detailed agent-based model for simulating the host:symbiont relationship between algal symbionts and sponges. We have demonstrated the ability of the model to produce realistic behavior when analyzed in the context of current knowledge about these relationships. For future work, we will explore which parameters have the largest effect on population size and growth rates of the symbiont populations, and will further investigate multiple-competitor and high-stress-environment scenarios. These are of interest to coral reef ecologists, and may identify field experiments that will shed light on the nature of the association between phototrophic symbionts and their heterotrophic hosts.

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REFERENCES

Canal-Vergés, P., M. Potthoff, F. T. Hansen, N. Holmboe, E. K. Rasmussen, and M. R. Flindt. 2014. "Eelgrass Re-establishment in Shallow Estuaries is Affected by Drifting Macroalgae: Evaluated by Agent-Based Modeling". *Ecological Modelling* 272:116–128.

Davy, S., D. Allemand, and V. Weis. 2012. "Cell Biology of Cnidarian-Dinoflagellate Symbiosis". *Microbiology and Molecular Biology Reviews* 76:229–261.

Day, T., L. Nagel, M. J. H. van Oppen, and M. J. Caley. 2008. "Factors Affecting the Evolution of Bleaching Resistance in Corals". *American Naturalist* 171 (2): E72–E88.

Hallock, P. 1981. "Algal Symbiosis: A Mathematical Analysis". *Marine Biology* 62:249–255.

Helbing, D., and S. Balietti. 2011. "How to Do Agent-Based Simulations in the Future: From Modeling Social Mechanisms to Emergent Phenomena and Interactive Systems Design". Technical Report 2011-06-024, Santa Fe Institute, Santa Fe, New Mexico. Available via http://www.santafe.edu/media/workingpapers/11-06-024.pdf [accessed 2 July 2015].

Hill, M. 2014. "Production Possibility Frontiers in Phototroph:Heterotroph Symbioses: Trade-offs in Allocating Fixed Carbon Pools and the Challenges These Alternatives Present for Understanding the Acquisition of Intracellular Habitats". *Frontiers in Microbiology* 5:357. doi:10.3389/fmicb.2014.00357.

Hill, M., A. Allenby, B. Ramsby, C. Schönberg, and A. Hill. 2011. "*Symbiodinium* Diversity Among Host Clionaid Sponges from Caribbean and Pacific Reefs: Evidence of Heteroplasmy and Putative Host-Specific Symbiont Lineages". *Molecular Phylogenetics and Evolution* 59:81–88.

Hill, M., and A. Hill. 2012. "The Magnesium Inhibition and Arrested Phagosome Hypotheses: New Perspectives on the Evolution and Ecology of *Symbiodinium* Symbioses". *Biological Reviews* 87:804–821.

Hill, M., and T. Wilcox. 1998. "Unusual Mode of Symbiont Acquisition After Bleaching in the Tropical Sponge *Anthosigmella varians*: Acquisition of Different Zooxanthellae Strains". *Symbiosis* 25:279–289.

Holland, J. N., D. L. DeAngelis, and J. L. Bronstein. 2002. "Population Dynamics and Mutualism: Functional Responses of Benefits and Costs". *American Naturalist* 159:231–244.

Muller, E., S. A. L. M. Kooijman, P. J. Edmunds, F. J. Doyle, and R. M. Nisbet. 2009. "Dynamic Energy Budgets in Syntrophic Symbiotic Relationships Between Heterotrophic Hosts and Photoautotrophic Symbionts". *Journal of Theoretical Biology* 259:44–57.

Pochon, X., M. Stat, M. Takabayashi, L. Chasqui, L. J. Chauka, D. D. K. Logan, and R. D. Gates. 2010. "Comparison of Endosymbiotic and Free-Living *Symbiodinium* (Dinophyceae) Diversity in a Hawaiian Reef Environment". *Journal of Phycology* 46:53–65.

Riesgo, A., K. Peterson, C. Richardson, T. Heist, B. Strehlow, M. McCauley, C. Cotman, M. Hill, and A. Hill. 2014. "Transcriptomic Analysis of Differential Host Gene Expression Upon Uptake of Symbionts: A Case Study with *Symbiodinium* and the Major Bioeroding Sponge *Cliona varians*". *BMC Genomics* 15:36. doi:10.1186/1471-2164-15-376.

Sachs, J. L., U. G. Mueller, T. P. Wilcox, and J. J. Bull. 2004. "The Evolution of Cooperation". *Quarterly Review of Biology* 79:135–160.

Scalera-Liaci, L., M. Sciscioli, E. Lepore, and E. Gaino. 1999. "Symbiotic Zooxanthellae in *Cinachyra tarentina*, a Non-Boring Demosponge". *Endocytobiosis and Cell Research* 13:105–114.

Spalding, M., C. Ravilious, and E. Green. 2001. *World Atlas of Coral Reefs*. Berkeley, CA: University of California Press. Prepared by the UNEP-World Conservation Monitoring Centre.

Stambler, N. 2011. "Marine Microalgae/Cyanobacteria-Invertebrate Symbiosis: Trading Energy for Strategic Material". In *All Flesh is Grass: Plant-Animal Interactions*, edited by J. Seckbach and Z. Dubinsky, Volume 16, 383–414. Springer.

Stoecker, D. K. 1998. "Conceptual Models of Mixotrophy in Planktonic Protests and Some Ecological and Evolutionary Implications". *European Journal of Protistology* 34:281–290.

Thornhill, D., Y. Xiang, W. Fitt, and S. Santos. 2009. "Reef Endemism, Host Specificity and Temporal Stability in Populations of Symbiotic Dinoflagellates from Two Ecologically Dominant Caribbean Corals". *PLoS ONE* 4 (7): e6262. doi:10.1371/journal.pone.0006262.

Weisz, J., A. Massaro, B. Ramsby, and M. Hill. 2010. "Zooxanthellar Symbionts Shape Host Sponge Trophic Status Through Translocation of Carbon". *Biological Bulletin* 219:189–197.

Wilkinson, C. 2008. *Status of Coral Reefs of the World: 2008*. Townsville, Australia: Global Coral Reef Monitoring Network and Reef and Rainforest Research Centre. 296 pp.

Yniguez, A. T., J. W. McManus, and D. L. DeAngelis. 2008. "Allowing Macroalgae Growth Forms to Emerge: Use of an Agent-Based Model to Understand the Growth and Spread of Macroalgae in Florida Coral Reefs, with Emphasis on *Halimeda tuna*". *Ecological Modelling* 216 (1): 60–74.

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