

1 LAGRANGIAN MICROBES: MIXING INDUCED ECOLOGICAL  
2 WARFARE

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7 **Abstract**

8 To investigate how submesoscale stirring in the ocean affects the biodiversity of  
9 marine microbial communities we utilize an agent-based modeling approach in which  
10 marine microbes are modeled as Lagrangian particles, termed *Lagrangian microbes*, that  
11 are advected by surface ocean currents derived from observations. Pairs of Lagrangian  
12 microbes interact once they are within some interaction length scale. For this preliminary  
13 investigation, the interaction is modeled using the neutral rock-paper-scissors game to  
14 ensure that no species is dominant. An efficient computational modeling framework  
15 has been developed allowing for the multi-year advection of millions of interacting  
16 Lagrangian microbes on distributed computing architectures. These simulations allow us  
17 to investigate the dynamics of microbial communities subject to diffusive, advective, and  
18 chaotic flows as well as real ocean currents (which exhibit all three).

19 We would like to emphasize that the majority of the work done so far has been in the  
20 development of this software package to efficiently advect millions of Lagrangian particles  
21 in 2D and 3D, efficiently resolve the interactions between all pairs of interacting microbes,  
22 handle arbitrary user-defined pairwise and self-interactions, and handle arbitrary microbe  
23 properties such as species and genetic information encoded as a binary string. In this  
24 sense, the project is at its beginning and we can now begin to use this software package to  
25 easily investigate the scientific questions of interest. Thus, only simple preliminary results  
26 are presented.

27 **1 Introduction**

28 Marine microbial communities serve an important role in mediating biogeochemical cycles  
29 and lie at the bottom of the oceanic food web sustaining all marine animal life. The geo-  
30 graphical structure of these microbial communities, and thus oceanic biodiversity, is set by  
31 short-range ecological interactions within submesoscale currents (Lévy et al., 2018).

32 For this preliminary investigation, we start off and focus on the North Pacific. In particular,  
33 we focus on the North Pacific subarctic-subtropical convergence zone shown in figure 1. This  
34 is a physically and biologically interesting region of the Pacific Ocean. The warmer and  
35 saltier subtropical gyre is more energetic with greater stirring rates and harbors more bio-  
36 diverse marine microbial communities. The colder and fresher subarctic gyre is less energetic  
37 and sustains a smaller variety of communities. In between the two gyres lies a transition  
38 zone. The frontal zones at the boundaries of the transition zone are dominated by mesoscale  
39 perturbation, especially on synoptic time scales.

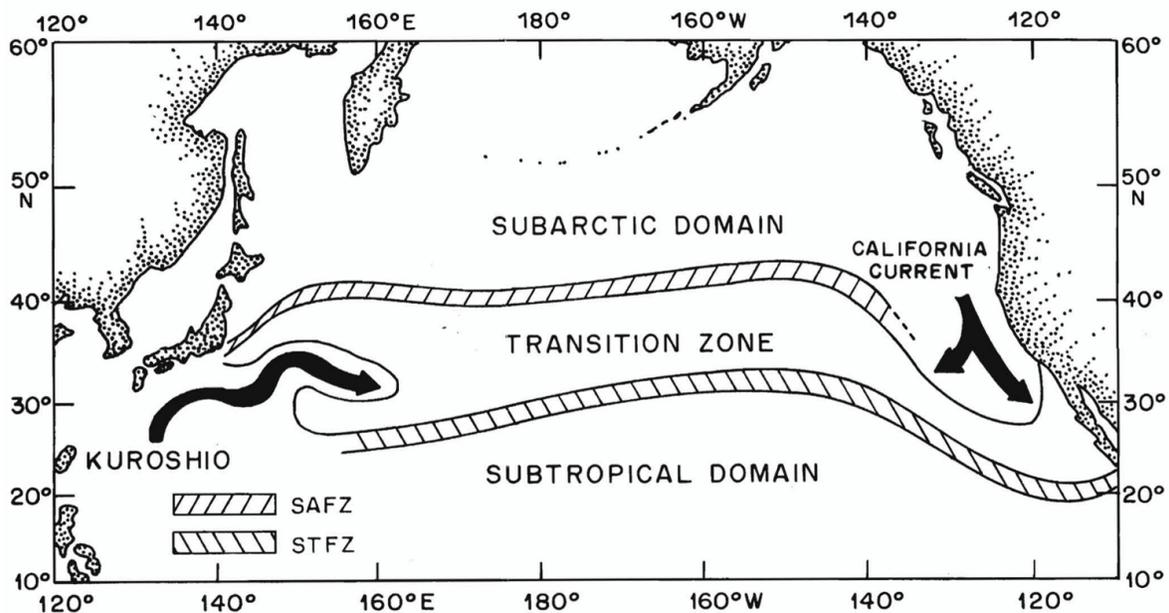


Figure 1: Schematic diagram of the North Pacific subarctic-subtropical convergence zone showing the locations of the subarctic and subtropical domains, the transition zone, and the associated subarctic frontal zone (SAFZ) and the subtropical frontal zone (STFZ). Black arrows indicate boundary current intrusions. Image credit: Roden (1991).

40 Numerous metrics can be used to quantify *stirring* in the global surface ocean. Among

41 them are the eddy kinetic energy, the strain rate, and finite-time Lyapunov exponents (FTLEs)  
42 (Vaugh and Abraham, 2008). We will focus on interpreting the latter. The FTLE of a velocity  
43 field at a point is a measure of how much time it would take for the trajectories of two  
44 infinitesimally close Lagrangian particles to diverge if they start at that point. The difference  
45 in activity between the subtropical and subarctic gyres can be seen in Lyapunov exponent  
46 based maps of ocean stirring. Figure 2 shows a snapshot of the finite-size Lyapunov exponent  
47 (FSLE) field in the North Pacific. The FSLE is similar to the FTLE but instead of measuring the  
48 time it would take the trajectories to diverge, it is a measure of the distance the two trajectories  
49 diverge by. The strongest feature is the extreme stirring occurring in the Kuroshio current. In  
50 the North Pacific, high levels of stirring can be seen in the subtropical domain with very low  
51 levels in the subarctic domain with a transition zone in between.

FSLEs based on the maximum eigenvalue of the Cauchy-Green strain tensor

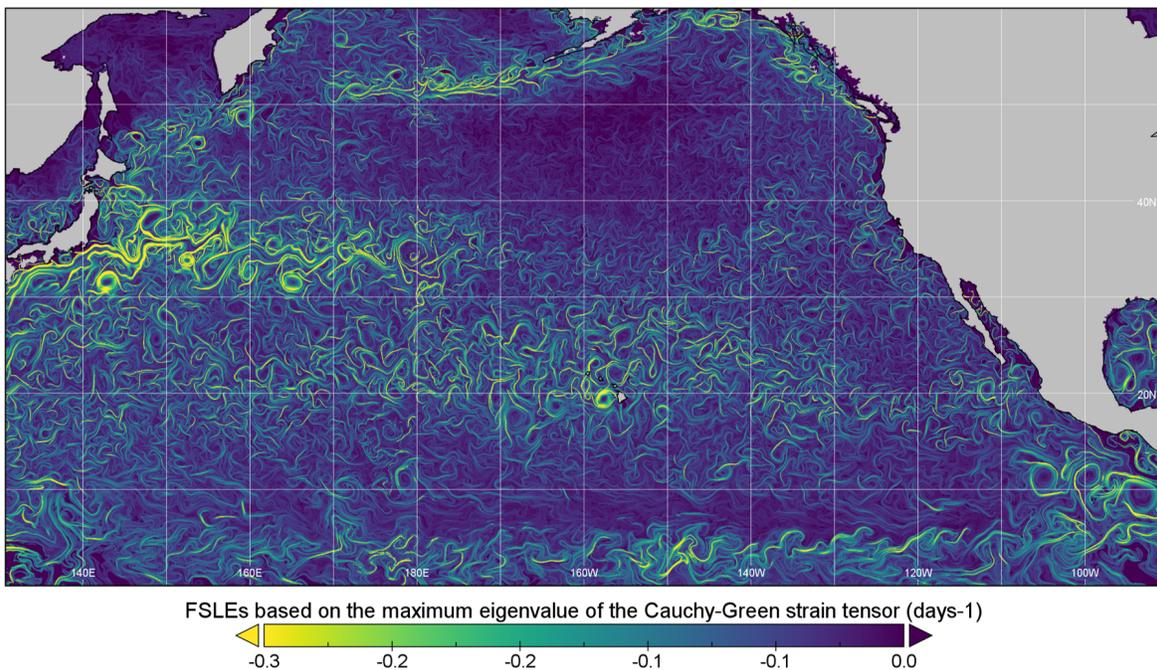


Figure 2: Snapshot of the finite-size Lyapunov exponent (FSLE) field in the North Pacific. Data obtained from the AVISO FSLE product.

52 Besides being a beautiful figure, the physical structures shown in figure 2 provides some  
53 motivation for this project. Streaks or filaments of strong stirring are visible with regions of  
54 low stirring on either sides of the streaks. Where stirring is strong we expect high competition  
55 between microbial species and high biodiversity. Where stirring is weak, we expect lower

56 levels of competition and lower levels of biodiversity.

57 Two fascinating questions we may ask ourselves are:

- 58 1. Is this submesoscale physical structure reflected in the biogeography of marine microbial  
59 communities?
- 60 2. Does it affect the dispersal of microbial species and the competitive dynamics between  
61 them?

62 With the advent of high-throughput DNA sequencing for oceanographic water samples it  
63 is a great time to be at the intersection of physical and biological oceanography to answer  
64 these questions. The biological composition of the ocean can be sampled at high spatial and  
65 temporal resolution providing a high-resolution picture of the biogeography of the oceans.  
66 This project focuses on computationally modeling these microbial communities and the  
67 competitive interactions between them in an idealized framework but with ocean currents  
68 derived from observations. The hope is to enable insights into the biogeography of the real  
69 ocean.

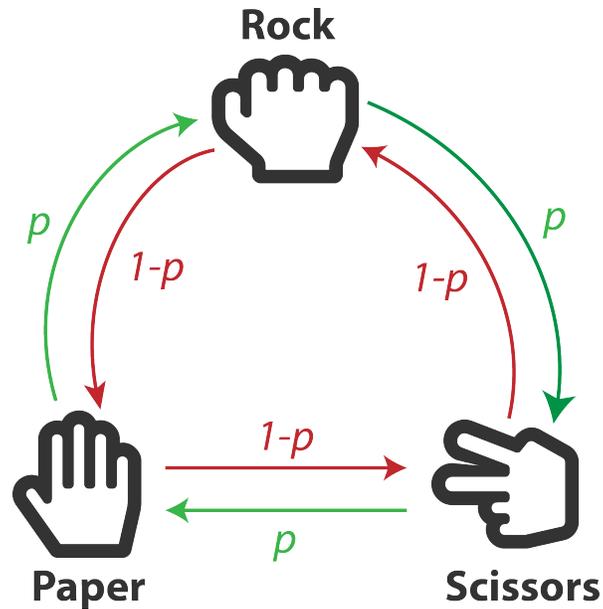


Figure 3: The modified rock-paper-scissors interaction played by the Lagrangian microbes. The forward interaction (green arrow) associated with the classical rock-paper-scissors game occurs with probability  $p$  while the *backward interaction* occurs with probability  $1 - p$ .

70 The pairwise interaction used here will a neutral rock-paper-scissors interaction. Figure 3

71 shows a schematic of this interaction. The interaction consists of two Lagrangian microbes  
72 playing rock-paper-scissors and the winner converts the losing microbe to its own species.  
73 This way the number of Lagrangian microbes  $N$  remains constant in time, which simplifies  
74 the simulation from a practical point of view as having Lagrangian microbes procreate and die  
75 means we have to regulate the total number of particles  $N$  to a reasonable number otherwise  
76 we risk overwhelming the simulation with too many particles, or having most of them die.  
77 The motivation behind using this interaction, besides being familiar to most children and  
78 readers, is that it ensures that no species is dominant. This reflects the observed *paradox of the*  
79 *plankton* (Hutchinson, 1961) where no plankton species appears to dominate the oceans even  
80 though dominant species appear in most terrestrial ecosystems.

## 81 **2 Computational methods and data used**

82 We take an agent-based modeling approach in which individual microbes are modeled as  
83 particles that are advected by the surface ocean currents in a Lagrangian particle tracking  
84 framework (van Sebille et al., 2018) using the Ocean Parcels package developed by Lange  
85 and van Sebille (2017).<sup>1</sup> The particle advection process was parallelized to allow for the fast  
86 advection of millions of particles. Advecting 490,000 particles for 8,760 time steps of 1 hour  
87 each (1 full year of simulation) takes 1 hour of wall clock time on 28 cores.

88 The near-surface ocean current velocity used to advect the Lagrangian microbes were  
89 provided by Earth Space Research (2009). The OSCAR (Ocean Surface Current Analysis  
90 Real-time) product contains near-surface ocean current estimates, derived using quasi-linear  
91 and steady flow momentum equations. The horizontal velocity is directly estimated from sea  
92 surface height, surface vector wind and sea surface temperature. The data were collected from  
93 the various satellites and in situ instruments. The model formulation combines geostrophic,  
94 Ekman and Stommel shear dynamics, and a complementary term from the surface buoyancy  
95 gradient. Data are interpolated onto a  $1/3^\circ$  grid with a 5-day temporal resolution.

96 Computing the interaction between pairs of Lagrangian microbes posed a slight challenge  
97 as a naive algorithm must check all  $N(N - 1)/2 \sim \mathcal{O}(N^2)$  pairs for a simulation consisting of  
98  $N$  Lagrangian microbes. The evaluation of pairwise interactions can be performed much more

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<sup>1</sup>Of course, we cannot hope to model all the individual microbe in the ocean so each agent in our model may perhaps represent a *super-organism* or microbial community or colony.

99 efficiently by storing the positions of each Lagrangian microbe in a  $k$ -d tree structure, which is  
100 a binary tree in which every leaf node is a  $k$ -dimensional point. Quadrees and octrees may be  
101 more familiar terms for this data structure in 2D and 3D respectively. Aluru (2018) provides a  
102 practical introduction to their use in computational science. We used the excellent and fast  
103  $k$ -d tree implementation provided by the SciPy module written in Cython (Jones et al., 2018)  
104 which uses the sliding midpoint rule of Maneewongvatana and Mount (1999) to perform the  
105 spatial partitioning in an optimal manner.

### 106 3 Preliminary results

107 We now present some results from a few simulations. We initialize 490,000 Lagrangian  
108 microbes with randomly assigned species (either rock, paper, or scissors) in a  $10^\circ \times 10^\circ$  box  
109 north of Hawaii (see the top panel of figure 4). After several thousand hours of advection  
110 and competitive interaction, a complex spatial and biogeographical structure emerges (see  
111 bottom panel of figure 4) that is reminiscent of the streaks in the FSLE field in figure 2. Certain  
112 isolated structures and filaments seem to be dominated by a single species while bulkier  
113 patches appear to be more biodiverse.

114 A simple statistic we can look at is the species count as a function of time, shown in figure  
115 5 for two values of  $p$  (0.9 and 0.55, see figure 3 for the definition of  $p$ ). Overall, each species  
116 seems to fluctuate around some quasi steady-state determined by the initial populations  
117 (approximately  $N/3$ ).

118 We note that for  $p = 0.9$  (top panel of figure 5) we still expect a neutral but more one-sided  
119 interaction as each species has one clear predator and one clear prey even though the prey  
120 may beat the predator with probability  $1 - p = 0.1$ . In this case the fluctuations are small (on  
121 the order of a few percent) and we interpret this as fierce competition between species. It is  
122 difficult for one species to dominate because if it grows in numbers, it will quickly end up  
123 in a region with a large number of predators and decrease in number. For  $p = 0.55$  (bottom  
124 panel of figure 5) the interaction is almost completely neutral as each species has one slight  
125 predator and one slight prey (they only beat their prey with probability  $p = 0.55$ ). In this case  
126 we see much larger and less frequent fluctuations in the species count. In this case because  
127 competition is much more random and two-sided, once a species grows in numbers it takes a  
128 while for the ecosystem to return to quasi-equilibrium.

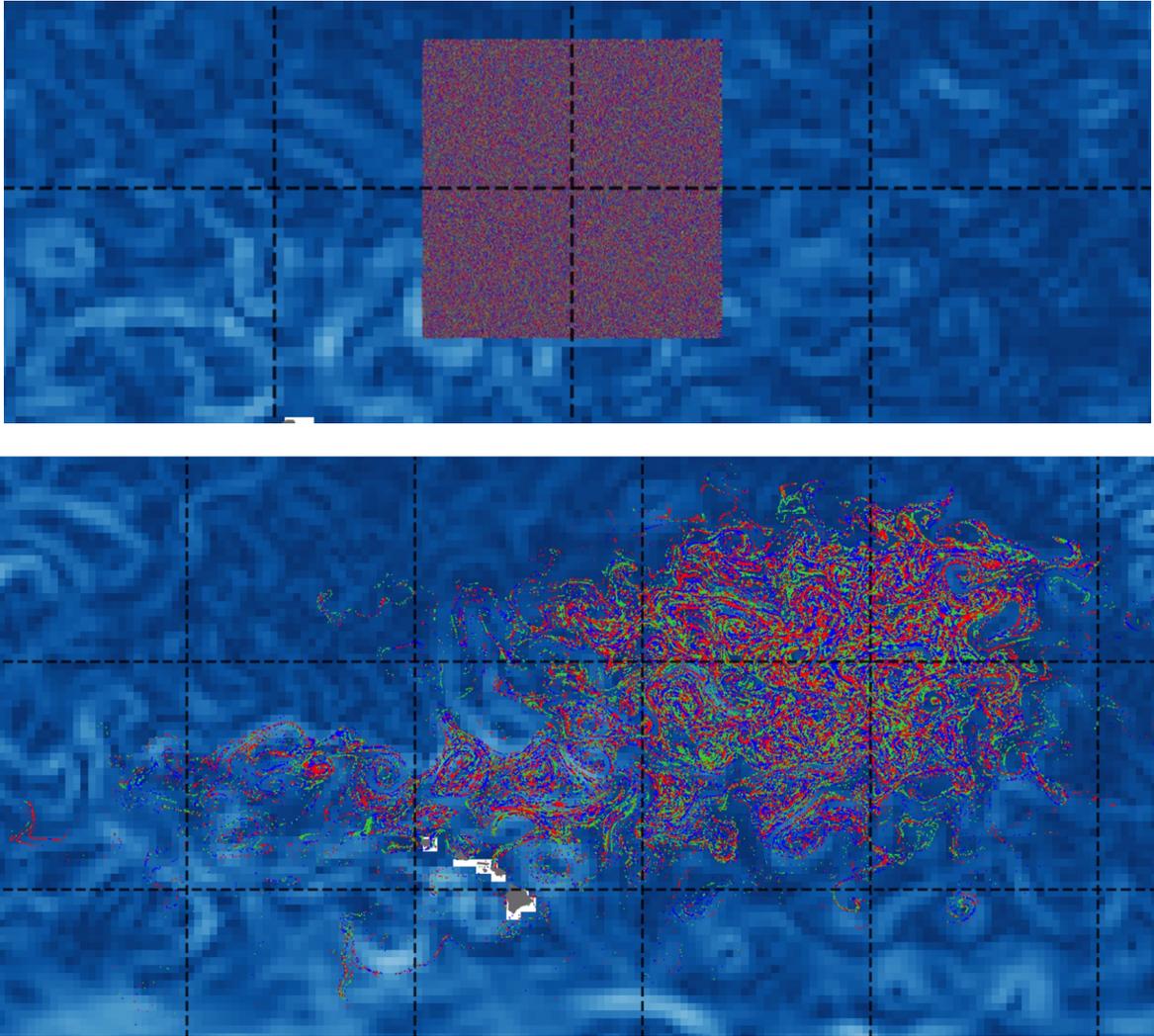


Figure 4: A snapshot of the simulation with  $p = 0.55$  at the initial time (top panel) and after several thousand hours (bottom panel). The different colors correspond to different species (either rock, paper, or scissors).

129 An interesting experiment we can carry out is to introduce an asymmetry in the rock-  
 130 paper-scissors interaction by varying one of the  $p$  values such as  $p_{RS}$ , the probability that  
 131 rock beats scissors, to introduce a dominant species. If  $p_{RS} > 0.5$  this should lead to the  
 132 exclusion of the scissors species. The species count for two such simulations where  $p_{RS}$  was  
 133 set to 0.6 and 0.51 are shown in figure 6. We see that with  $p_{RS} = 0.6$  the scissors population is  
 134 excluded extremely quickly. The  $e$ -folding time scale associated with their exclusion across  
 135 the Pacific gives an *exclusion time scale* of 250 hours, or roughly 10 days. This is unrealistically  
 136 fast. Interesting, if  $p_{RS}$  is reduced to 0.51 to provide a slight imbalance, then the exclusion still

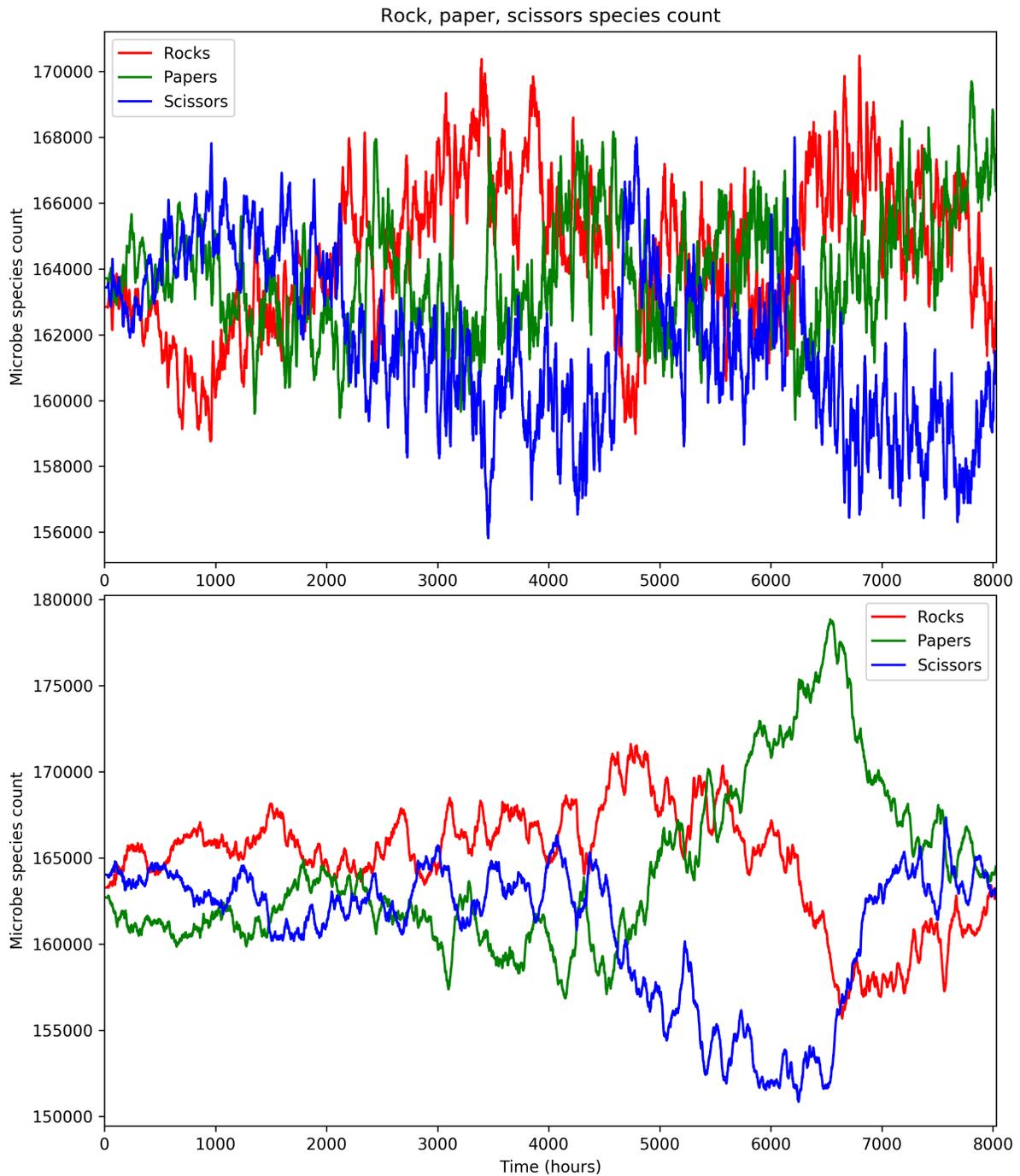


Figure 5: Species count as a function of time for simulations with  $p = 0.9$  (top) and  $p = 0.55$  (bottom) where 490,000 regularly spaced Lagrangian microbes were initialized in a small patch with randomly assigned initial species. The overall system seems to fluctuate around some quasi steady-state determined by the initial populations (approximately  $490,000/3$ ).

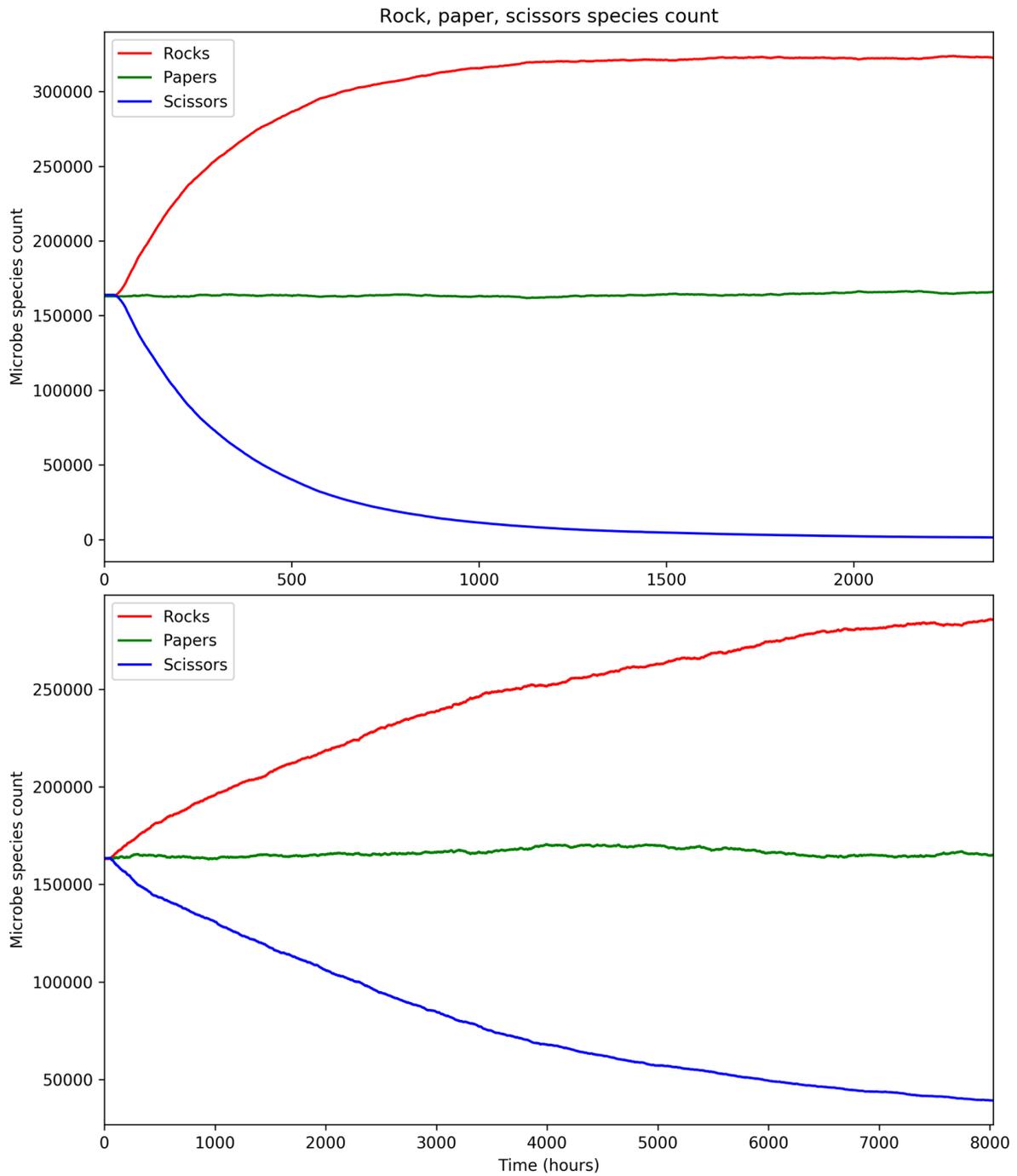


Figure 6: Species count as a function of time for simulations with  $p_{RS} = 0.6$  (top) and  $p_{RS} = 0.51$  (bottom) where 490,000 regularly spaced Lagrangian microbes were initialized in a small patch with randomly assigned initial species.

137 occurs but with an  $e$ -folding time scale of 2500 hours or roughly 104 days: an increase by a  
 138 factor of 10 for a decrease of a factor of 10 towards neutrality for  $p_{RS}$ .

## 139 4 Future work and preliminary conclusions

140 Unfortunately most of the time was spent on code development, and the interesting investi-  
141 gations we wish to carry out lie in the future. Here we include a laundry list, or perhaps a  
142 rambling list, of topics of future investigation and improvement.

143 Immediate future work will be to investigate the cross-species pairwise distance his-  
144 tograms which should provide greater insight into the effect of the interaction on the patch  
145 sizes. They are apparently referred to as spatial heterozygosity plots in the theoretical ecology  
146 literature, or a spatial variogram in geostatistics. These would also provide insight into the  
147 spatial structure of the Lagrangian microbes and their biogeography, which can then be  
148 compared with the spatial patterns in the FSLE fields (figure 2).

149 The current simulations only include advection and do not account for stochastic motions.  
150 Adding diffusion terms would be interesting to investigate the effect of low and high dif-  
151 fusivity on competition and biogeography. Here we expect low diffusivities to wiggle the  
152 Lagrangian microbes around their trajectories while a high diffusivity may kick the microbes  
153 out of eddies leading to lower levels of competition perhaps.

154 To get closer to answering the question of biodiversity in the ocean, a quantitative measure  
155 of biodiversity is needed. This may be provided by the  $\beta$ -diversity or the Shannon diversity  
156 index calculated over prescribed bins throughout the simulation domain.

157 We think a further modification to the rock-paper-scissors game in which the forward  
158 interaction occurs with probability  $p$  and the backward interaction occurs with probability  
159  $q$  so that  $p + q < 1$  and  $1 - p - q$  is the probability that no interaction occurs would be  
160 an improvement that dampens unphysical fast-moving *ecological waves* due to cascading  
161 interactions that occur over successive time steps.

162 A common topic of fun discussion and potential investigation is the evolution of microbial  
163 populations in Agulhas rings which are coherent warm core ring structures that get pinched  
164 off the Agulhas current as it flows from the Indian to the Atlantic Ocean south of Africa.

165 The simulations we presented are performed on a two-dimensional ocean surface and  
166 inevitably motivate the need for investigations to consider the fundamentally different three-  
167 dimensional nature of the real ocean and the effect of diurnal vertical migration on competition  
168 and biogeography.

169 An exciting avenue of research motivated by recent work by [Plummer et al. \(2018\)](#) in

170 which competition between biological species in marine environments is investigated by  
171 means of an agent-based model on a one-dimensional grid with a focus on how weakly  
172 compressible flows affect fixation probabilities. They suggest that even weak convergences  
173 or divergences of water masses can bring together or disperse microbial communities which  
174 affects competition and survivability much more than diffusion or advection. We intend  
175 to investigate the relationship between regions of convergence and divergence in observed  
176 surface ocean velocities, perhaps by populating a region of high divergence with Lagrangian  
177 microbes of one species and tracking their future success.

178 The list of potential scientific questions that may be investigated in this framework seems  
179 to be exponentially increasing with the number of discussions had, which may explain why  
180 this type of agent-based modeling has been incredibly popular in theoretical ecology.

## 181 **Acknowledgements**

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188 stack (Oliphant, 2007; Millman and Aivazis, 2011; Jones et al., 2018), Jupyter Lab (Pérez and  
189 Granger, 2007; Kluyver et al., 2016), xarray (Hoyer and Hamman, 2017), matplotlib (Hunter,  
190 2007), Cartopy (Met Office, 2018), cmocean (Thyng et al., 2016).

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