

LAGRANGIAN MICROBES: MIXING INDUCED ECOLOGICAL WARFARE

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Abstract

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

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

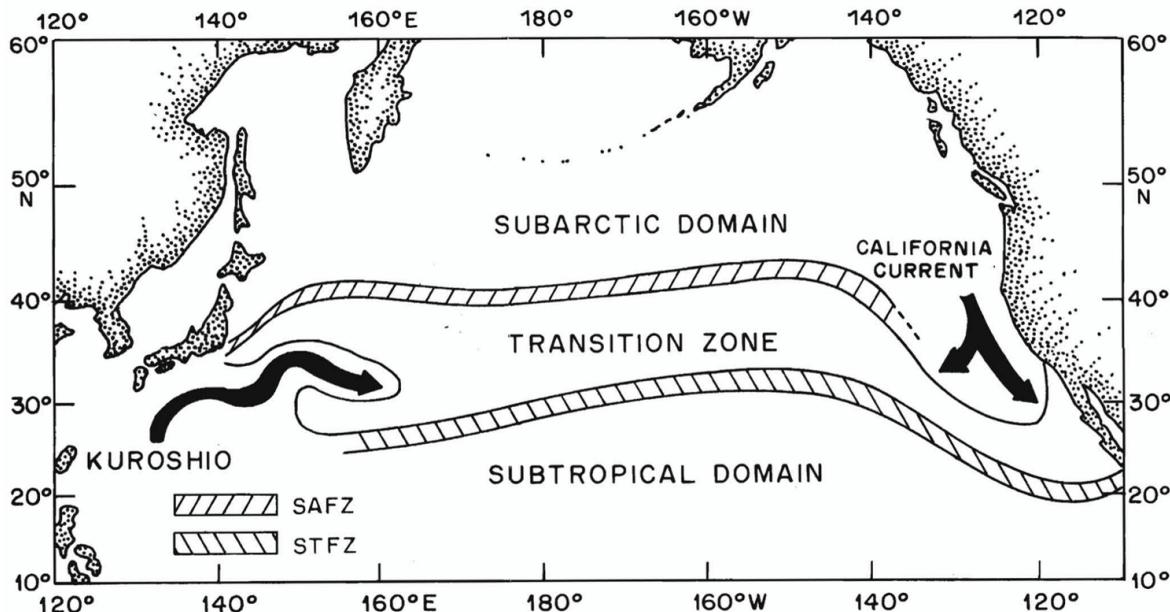


Figure 1: Schematic diagram of the North Pacific subarctic-subtropical convergence zone showing the locations of the subarctic and subtropical domains, the transition zone, and the associated subarctic frontal zone (SAFZ) and the subtropical frontal zone (STFZ). Black arrows indicate boundary current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

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

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

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

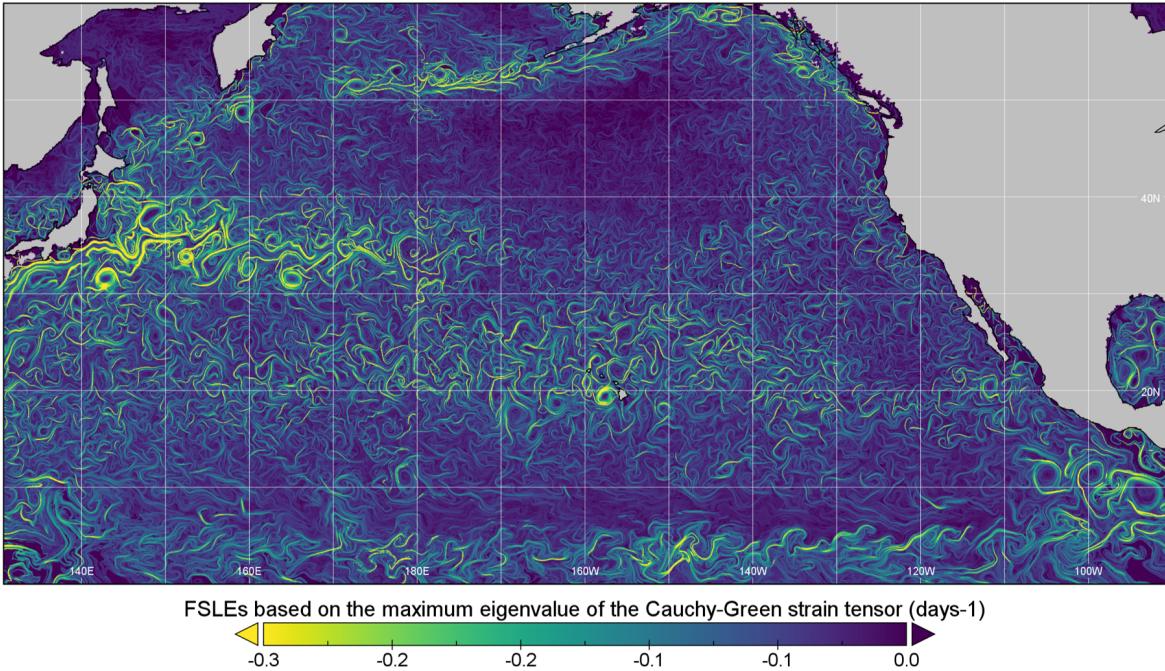


Figure 2: Snapshot of the finite-size Lyapunov exponent (FSLE) field in the North Pacific. Data obtained from the AVISO FSLE product.

Besides being a beautiful figure, the physical structures shown in figure 2 provides some motivation for this project. Streaks or filaments of strong stirring are visible with regions of low stirring on either sides of the streaks. Where stirring is strong we expect high competition 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.

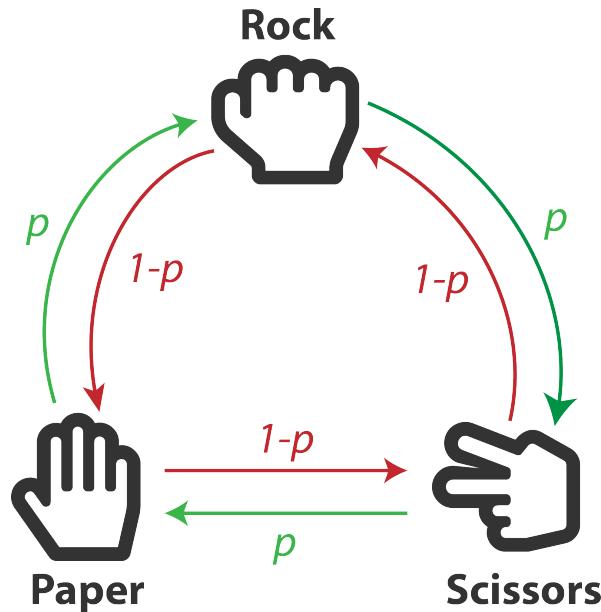


Figure 3: The modified rock-paper-scissors interaction played by the Lagrangian microbes. The forward interaction (green arrow) associated with the classical rock-paper-scissors game occurs with probability p while the *backward interaction* occurs with probability $1 - p$.

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).¹ 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

¹Of 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. Quadtrees 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.

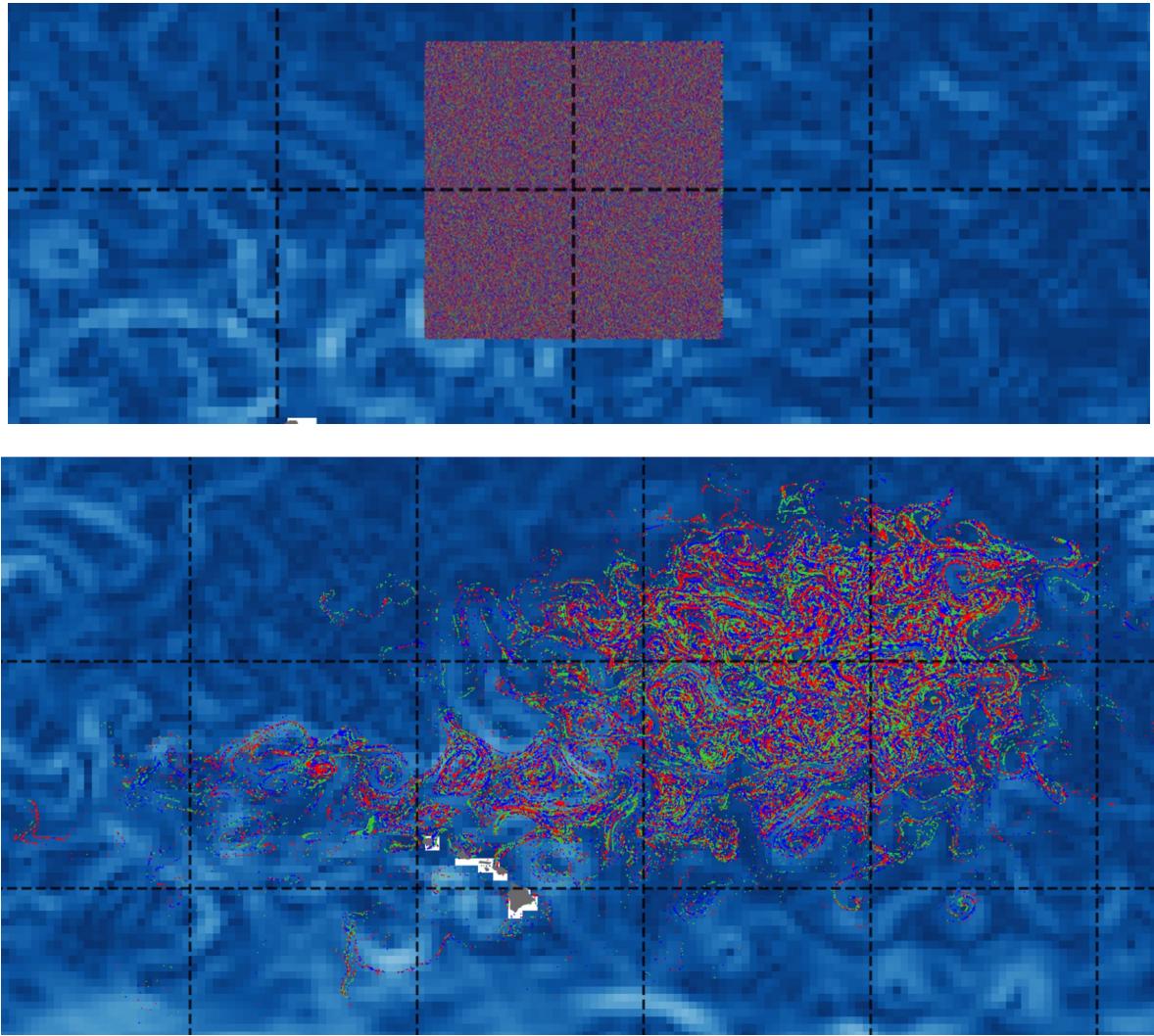


Figure 4: A snapshot of the simulation with $p = 0.55$ at the initial time (top panel) and after several thousand hours (bottom panel). The different colors correspond to different species (either rock, paper, or scissors).

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

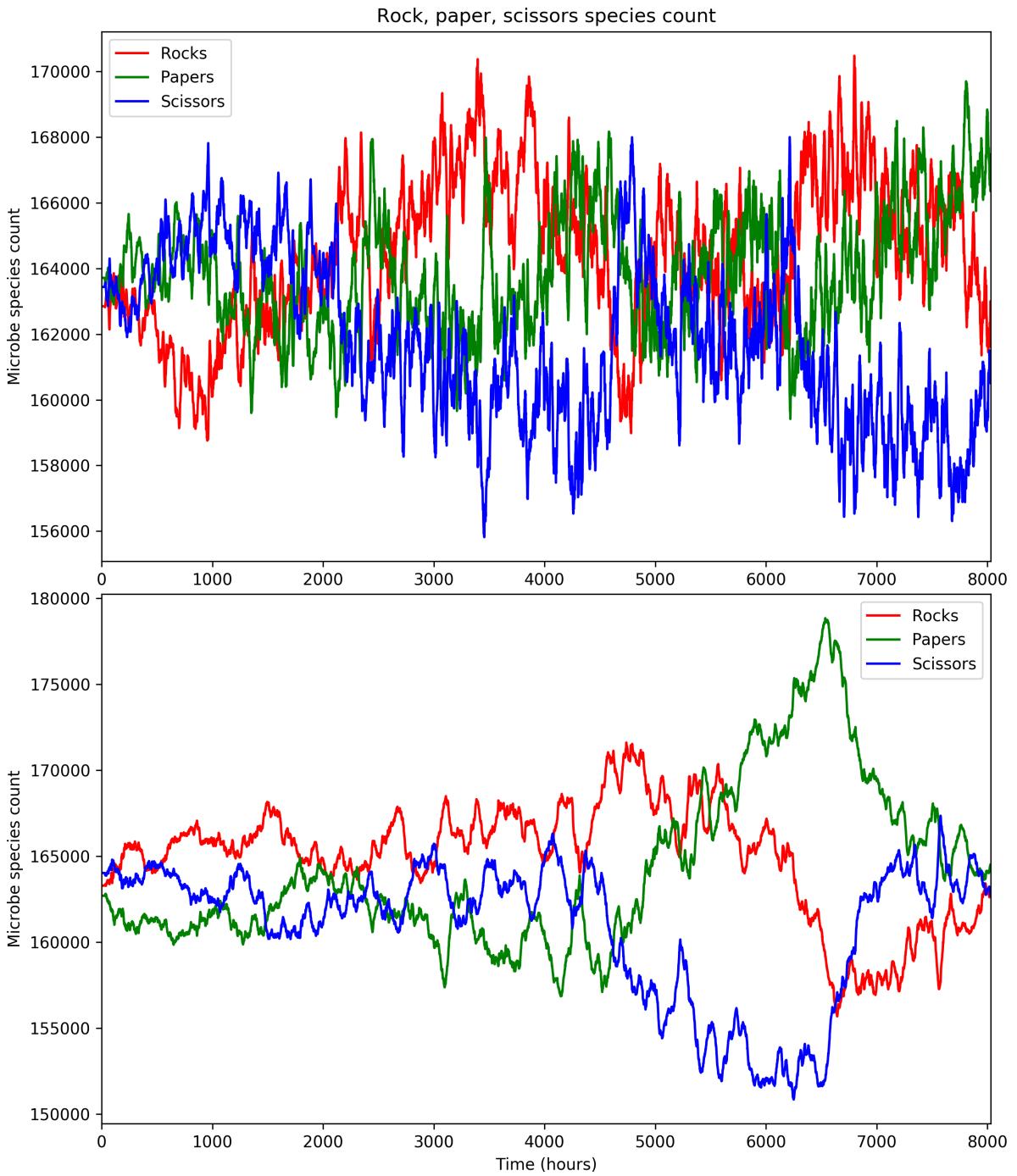


Figure 5: Species count as a function of time for simulations with $p = 0.9$ (top) and $p = 0.55$ (bottom) where 490,000 regularly spaced Lagrangian microbes were initialized in a small patch with randomly assigned initial species. The overall system seems to fluctuate around some quasi steady-state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

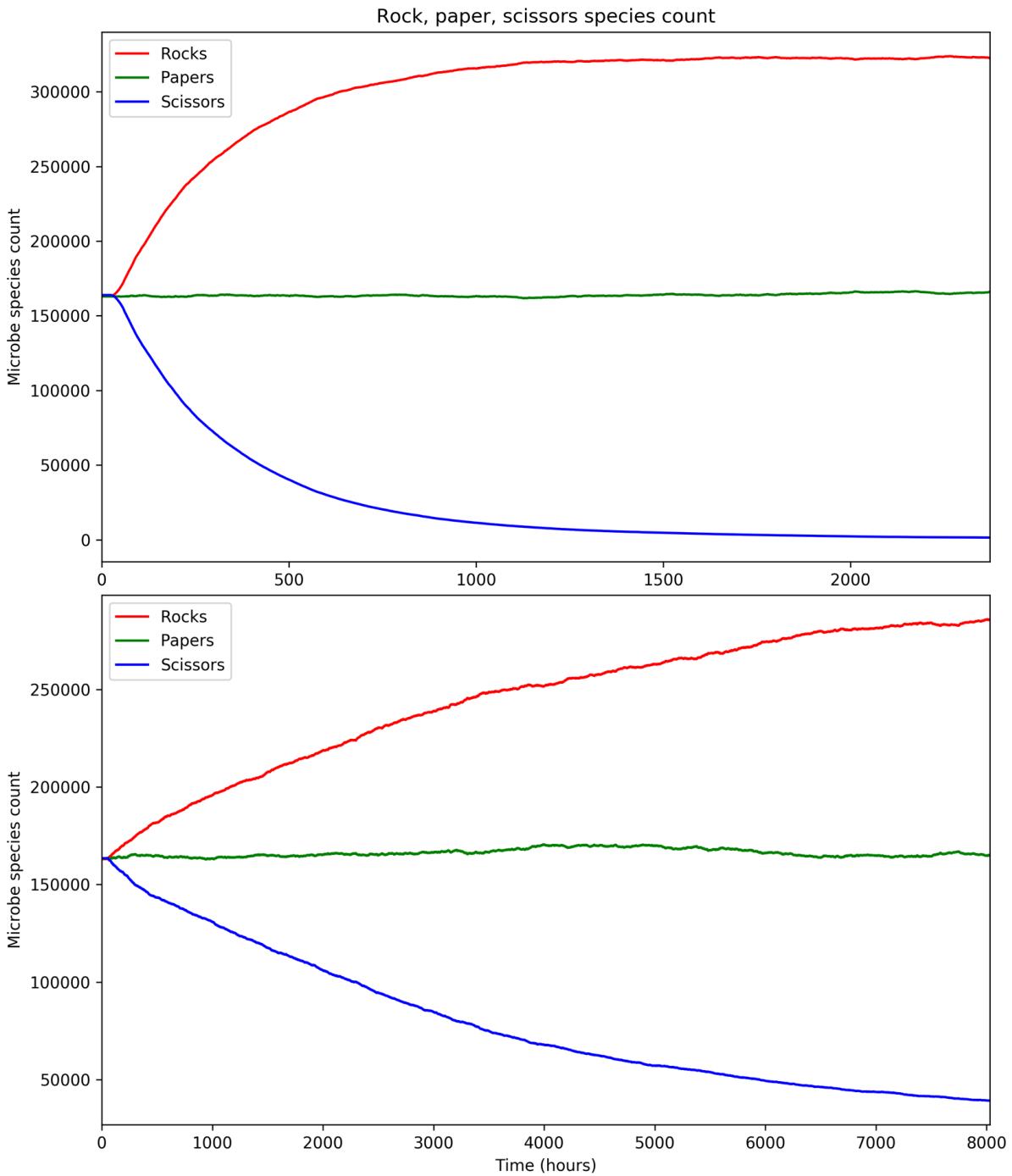


Figure 6: Species count as a function of time for simulations with $p_{RS} = 0.6$ (top) and $p_{RS} = 0.51$ (bottom) where 490,000 regularly spaced Lagrangian microbes were initialized in a small patch with randomly assigned initial species.

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 β -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

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

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

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References

- Aluru, S. (2018). Quadtrees and Octrees. In Mehta, D. P. and Sahni, S., editors, *Handbook of Data Structures and Applications, 2nd edition*, pages pp. 309–327. Chapman and Hall/CRC, Boca Raton, Florida.
- Bezanson, J., Edelman, A., Karpinski, S., and Shah, V. B. (2017). Julia: A fresh approach to numerical computing. *SIAM review*, 59(1):65–98.
- Earth Space Research (2009). Oscar third degree resolution ocean surface currents. version 1.

- 198 Dataset accessed [2018-09-25] at <http://dx.doi.org/10.5067/OSCAR-03D01>.. PO.DAAC,
199 CA, USA.
- 200 Hoyer, S. and Hamman, J. (2017). xarray: N-D labeled arrays and datasets in Python. *Journal
201 of Open Research Software*, 5(1).
- 202 Hunter, J. D. (2007). Matplotlib: A 2D graphics environment. *Computing In Science & Engineer-
203 ing*, 9(3):90–95.
- 204 Hutchinson, G. E. (1961). The Paradox of the Plankton. *The American Naturalist*, 95(882):137–
205 145.
- 206 Jones, E., Oliphant, T., Peterson, P., et al. (2018). SciPy: Open source scientific tools for Python.
207 [Online; accessed December 5, 2018].
- 208 Kluyver, T., Ragan-Kelley, B., Pérez, F., Granger, B., Bussonnier, M., Frederic, J., Kelley, K.,
209 Hamrick, J., Grout, J., Corlay, S., Ivanov, P., Avila, D., Abdalla, S., and Willing, C. (2016).
210 Jupyter notebooks – a publishing format for reproducible computational workflows. In
211 Loizides, F. and Schmidt, B., editors, *Positioning and Power in Academic Publishing: Players,
212 Agents and Agendas*, pages 87 – 90. IOS Press.
- 213 Lange, M. and van Sebille, E. (2017). Parcels v0.9: prototyping a lagrangian ocean analysis
214 framework for the petascale age. *Geoscientific Model Development*, 10(11):4175–4186.
- 215 Lévy, M., Franks, P. J., and Smith, K. S. (2018). The role of submesoscale currents in structuring
216 marine ecosystems. *Nature communications*, 9(1):4758.
- 217 Maneewongvatana, S. and Mount, D. M. (1999). It's okay to be skinny, if your friends are fat.
218 In *Center for Geometric Computing 4th Annual Workshop on Computational Geometry*, volume 2,
219 pages 1–8.
- 220 Met Office (2010 - 2018). *Cartopy: a cartographic python library with a matplotlib interface*. Exeter,
221 Devon.
- 222 Millman, K. J. and Aivazis, M. (2011). Python for scientists and engineers. *Computing in
223 Science & Engineering*, 13(2):9–12.
- 224 Oliphant, T. E. (2007). Python for scientific computing. *Computing in Science & Engineering*,
225 9(3).

- 226 Pérez, F. and Granger, B. E. (2007). IPython: a system for interactive scientific computing.
227 *Computing in Science and Engineering*, 9(3):21–29.
- 228 Plummer, A., Benzi, R., Nelson, D. R., and Toschi, F. (2018). Fixation probabilities in weakly
229 compressible fluid flows. *arXiv preprint arXiv:1808.07128*.
- 230 Roden, G. I. (1991). Subarctic-subtropical transition zone of the North Pacific: large-scale
231 aspects and mesoscale structure. *NOAA Technical Report NMFS*, 105:1–38.
- 232 Thyng, K. M., Greene, C. A., Hetland, R. D., Zimmerle, H. M., and DiMarco, S. F. (2016).
233 True colors of oceanography: Guidelines for effective and accurate colormap selection.
234 *Oceanography*, 29(3):9–13.
- 235 van Sebille, E., Griffies, S. M., Abernathey, R., Adams, T. P., Berloff, P., Biastoch, A., Blanke,
236 B., Chassignet, E. P., Cheng, Y., Cotter, C. J., Deleersnijder, E., Döös, K., Drake, H. F.,
237 Drijfhout, S., Gary, S. F., Heemink, A. W., Kjellsson, J., Koszalka, I. M., Lange, M., Lique,
238 C., MacGilchrist, G. A., Marsh, R., Adame, C. G. M., McAdam, R., Nencioli, F., Paris, C. B.,
239 Piggott, M. D., Polton, J. A., Rühs, S., Shah, S. H., Thomas, M. D., Wang, J., Wolfram, P. J.,
240 Zanna, L., and Zika, J. D. (2018). Lagrangian ocean analysis: Fundamentals and practices.
241 *Ocean Modelling*, 121:49–75.
- 242 Waugh, D. W. and Abraham, E. R. (2008). Stirring in the global surface ocean. *Geophysical
243 Research Letters*, 35(20).