

1 MicroxanoX: an R package for simulating an aquatic
2 *MIC*Robial ecosystem that can occupy *OX*ic or
3 *ANOX*ic states.

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5 **Abstract**

Ca. 100 words.

6 *Keywords:* reproducibility; regime shift;, reproducibility; regime shift;

7 **1. TODO**

- 8 • **update links**
9 • **update cross references**
10 • **check keywords**
11 • **add more references**
12 • **expand on Impact and Conclusion section**

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13 2. Required Metadata

14 2.1. Current code version

15 Ancillary data table required for subversion of the codebase.

Nr.	Code metadata description	Please fill in this column
C1	Current code version	v0.9.0
C2	Permanent link to code/repository used for this code version	https://github.com/UZH-PEG/microxanox
C3	Code Ocean compute capsule	
C4	Legal Code License	CC BY 4.0
C5	Code versioning system used	git
C6	Software code languages, tools, and services used	R
C7	Compilation requirements, operating environments	R (>= 4.1.0) magrittr tibble ggplot2 patchwork grDevices stats mgcv deSolve dplyr tidyr stringr multidplyr
C8	If available Link to developer documentation/manual	TO BE ADDED
C9	Support email for questions	Rainer.Krug@uzh.ch; Rainer@krugs.de

16 3. Motivation and significance

17 Mathematical models play a key role in the development of understanding
 18 about how ecosystems work and how they respond to environmental changes
 19 [1, 3, 13]. They are also critical for developing hypotheses that can then be
 20 tested in experimental studies. One area of ecology in which simple models have

21 played a very influential role is the area of how ecosystems respond to gradual
22 environmental change [8]. - Scheffer, M., Carpenter, S., Foley, J. a, Folke, C. &
23 Walker, B. (2001). Catastrophic shifts in ecosystems. Nature, 413, 591–6.

24 It is conceivable that an ecosystem state, such as the total biomass of a
25 particular type of bacteria, may remain unchanged when something about its
26 environment changes, such as the temperature. It is possible that the ecosystem
27 state changes gradually itself. It is also possible that the ecosystem state may
28 change abruptly into a new state that is difficult to recover from [9].

29 This possibility for abrupt, perhaps catastrophic changes that are difficult to
30 reverse causes considerable concern [4, 6, 12].

31 An example where the gradual change of a single environmental variable is
32 causing an abrupt change of the system is the switch from an aerobic (oxygen is
33 available for metabolism) to anaerobic (oxygen generally unavailable) system.
34 This system has been investigated by Bush et al. [2] in a simulation study of
35 a mathematical model of the system. They showed that gradual change in the
36 environment could cause catastrophic changes in the ecosystem state that would
37 be difficult to reverse.

38 One limitation of the study by Bush et al. [2] was limited biodiversity in the
39 ecosystem model. Specifically, there were three functional groups of bacteria,
40 but within each of these groups, there was no biodiversity. This then leaves open
41 the question of if and how biodiversity within functional groups, in their model,
42 affects the ecosystem response to environmental change. This limitation is not
43 limited to the study of Bush et al. [2], there are few if any studies of the effects
44 of biodiversity on abrupt transitions between ecosystem states.

45 We decided to fill this research gap, by making a simulation study of how
46 within functional group biodiversity affects ecosystem responses to environmental
47 change Limberger [5], and to base our work on the work and model of Bush et al.
48 [2]. It was with this goal in mind that we developed the *microxanox* package.
49 The first stage of development was to write code from scratch (as there was
50 no available code to start from) and to confirm that this new implementation
51 would reproduce the previously published results. The resulting reproduction is
52 available as one of the package vignettes: [vignette Partial reproduction of Bush](#)
53 [et al.](#)

54 The second stage was to add functionality that would be necessary to answer
55 our research question. Most importantly, we made it possible to have multiple
56 species of bacteria within each of the three functional groups, for the multiple
57 species to differ in their characteristics, and to vary the number of species and
58 amount of variability among them. We also added functionality that allowed:
59 temporally varying environmental conditions, addition of random noise to state
60 variables, and immigration. In addition to the model itself, the package includes
61 some functions to analyse the results as well as visualize the results to provide
62 a starting point for customized visualizations based on own requirements. The
63 basic and additional functionality is described in the package [User Guide](#).

64 4. Software description

65 {»Describe the software in as much as is necessary to establish a
66 vocabulary needed to explain its impact.«}

67 The *microxanox* package is for simulating a three functional group system
68 (*CB*: cyanobacteria, *PB*: phototrophic sulfur bacteria, and *SB*: sulfate-reducing
69 bacteria) with four chemical substrates (*P*: phosphorus, *O*: oxygen, *SR*: reduced
70 sulfur, *SO*: oxidized sulfur). It includes feedback between biogeochemical pro-
71 cesses and is based on Bush et al. [2] (See Bush et al. [2] for a detailed discussion
72 of the model). At the core of the simulations is a set of ordinary differential
73 equations (specified in the function `bushplus_dynamic_model()`, though users
74 do not need to call this function directly). There are functions for running
75 individual simulations and for running a set of simulations across, for example,
76 a range of environmental conditions.

77 To make the simulation run with multiple species, we expressed different
78 species characteristics in the elements of vectors and matrices. We also adapted
79 the code for the ordinary differential equations to include the vectors and
80 matrices, and to use matrix mathematics. In this way, we made it possible to
81 run simulations with different numbers of species without having to change the
82 underlying code.

83 The package functions and code are structured in modular, so that some
84 new functionality can be easily added. E.g. the event definition can easily be
85 changed, or other aspects can be adjusted. All values in the parameter object
86 can be changed as needed and the general structure of the code should make it
87 not too difficult to adapt the model to other similar systems.

88 4.1. Software architecture

89 {»Give a short overview of the overall software architecture; provide
90 a pictorial component overview or similar (if possible). If necessary
91 provide implementation details.«}

92 The framework used when writing this package aimed to maximise simplicity
93 for the user, and to make it easy to reproduce results (see the supplement to
94 Limberger [5] for an example of how this is used). As such, all the parameters
95 needed to run a simulation or find a stable state are contained in a single
96 object (which can easily be created using included functions). This parameter
97 object is given to a function that runs the simulations and returns the results.
98 The returned results object is identical to the parameter object but with an
99 additional slot named `results`, which contains the results of the run. Thus
100 the returned results object contains the simulation conditions (parameters) as
101 well as the results, and can be used to run the simulation again. This promotes
102 reproducibility and makes incremental changes of individual parameters and
103 re-running the simulations straightforward.

104 In the following sections we describe how to use the package to run one
105 simulation and to find steady states across an environmental gradient.

106 4.2. Running one simulation

107 A typical simulation would look as shown in @ref(fig:runsim_example).

108 A simulation is run using the `run_simulation()` function. In this function,
109 the ODEs are solved using the function `ode()` in the package *deSolve* package [11].
110 The `run_simulation()` function needs only one argument - an object as created
111 by the function `new_runsim_parameter()`. The parameter object returned by
112 `new_runsim_parameter()` contains among other things the `strain_parameter`
113 object, which can be created by the function `new_strain_parameter()`. For
114 a detailed description of the parameter objects, their meaning and how they
115 are created and have values set and changed please see the *User Guide* which
116 accompanies the package or is available at [User Guide](#)

117 After the parameter object has been defined, it can be used in the `run_simulation()`
118 function. The function returns an object which is identical to the parameter
119 object, except of an additional slot containing the results. This design produces
120 a fully reproducible object as it can be used as a parameter object to be fed
121 back into the `run_simulation()` function to run the simulation again from the
122 parameter used to generate the results before.

123 4.3. Finding Steady States

124 The general approach used to find the stable state of the system with a
125 specific parameter set is to run the simulation for a long time and record the
126 final state. When one does this across a range of environmental conditions, one
127 discovers how the steady state of the system responds to the environmental
128 conditions. The package contains functionality for finding steady states that
129 correspond to values of one environmental variable, namely the value of oxygen
130 diffusivity.

131 Two methods for finding steady states are implemented. The first runs a
132 separate simulation for each combination of starting conditions and oxygen
133 diffusivity (let us term this the *Replication method*). This is the method used
134 in the Bush et al. [2] study. The second runs only two simulations, with step-
135 wise and slowly temporally increasing oxygen diffusivity, and the other with
136 step-wise and slowly decreasing or decreasing oxygen diffusivity. During this
137 temporal environmental change, the state of the system was recorded just before
138 change to a new oxygen diffusivity (let us term this the *Temporal method*). We
139 implemented two methods since there is no definitive best method, and in order
140 to check if results were sensitive to choice of method.

141 The replication method is implemented in the function `run_replication_ssfind()`
142 which takes a parameter object as returned by the function `new_replication_ssfind_parameter()`
143 and the number of cores for multithreading the simulation. As the multithreading
144 uses the package function `mclapply()` from the package `parallel` [7], the mult-
145 threading only works on Linux and Mac. It is planned to move to `parLapply()`
146 [7] in a future release.

147 This temporal method implemented in the function `run_temporal_ssfind()`,
148 which takes a parameter object as created by the function `new_temporal_ssfind_parameter()`.
149 It is planned for a later release, to run these two simulations in parallel.

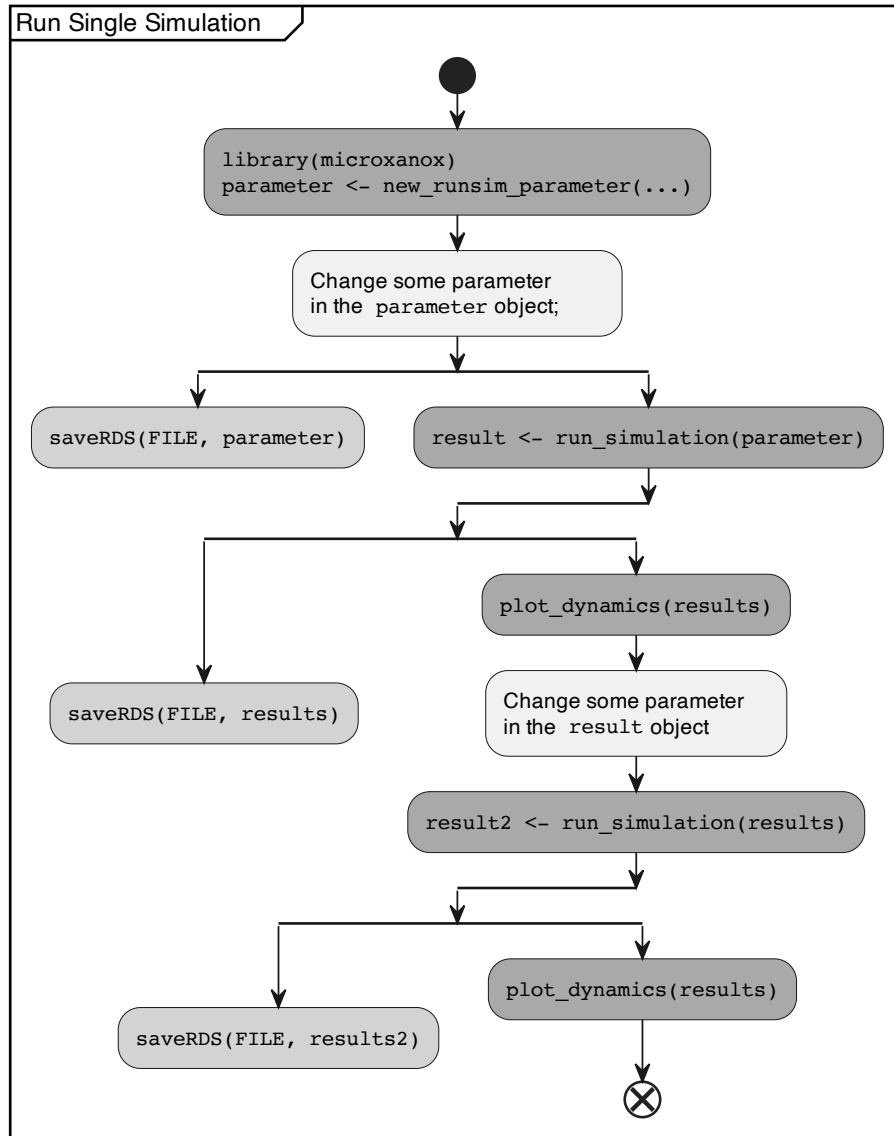


Figure 1: Typical flow of a simulation. Dark Grey boxes: commands necessary for simulation; Light Grey: Saving of parameter and results; Lightest Grey: Different non specified commands.

150 For a more detailed walk-through of these two approaches and explanation
151 please see the [User Guide](#).

152 4.4. *Visualising and analysing results*

153 From the raw results returned, summary measures about how the ecoys-
154 tem stable states respond to environmental change can be extracted. The
155 function `get_stability_measures()` returns quantities such as the amount of
156 environmental change required for the system to abruptly change to a different
157 state.

158 The function `plot_dynamics()` plots a single simulation run, as returned from
159 the `run_simulation()` function. This function is only provided as a convenience
160 function to provide a way to easily see the results of a simulation run. An
161 example plot resulting from this function is shown in @ref(fig:plot-dynamics).

162 5. Impact

163 { »This is the main section of the article and the reviewers weight the
164 description here appropriately Indicate in what way new research
165 questions can be pursued as a result of the software (if any). Indicate
166 in what way, and to what extent, the pursuit of existing research
167 questions is improved (if so). Indicate in what way the software
168 has changed the daily practice of its users (if so). Indicate how
169 widespread the use of the software is within and outside the intended
170 user group. Indicate in what way the software is used in commercial
171 settings and/or how it led to the creation of spin-off companies (if
172 so).« }

173 The free and open source implementation and extension of the model used
174 in Bush et al. [2] provides the means of reproducing the results published while
175 at the same time provides the means of doing unique, innovative, and important
176 investigations of how ecosystems respond to environmental change. The design
177 of the package code and functionality is with reproducibility in mind: the
178 combination of all parameters being in a single parameter object as well as the
179 return of the simulation as a result object which inherits from the parameter
180 object provides a relatively easy to use framework to implement reproducible
181 experiments.

182 While the package was not intended to provide a code which can be very
183 easily adapted to other types of ecosystems and types of organism, it seems
184 likely that the overall framework could be used as a basis for models of other
185 ecosystems and organisms. For example, all such models would have parameters
186 that differ among species and need to be described in an object. All would
187 need to run simulations and sets of simulations across environmental conditions.
188 Researchers want to model a new ecosystem do not, therefore, have to start from
189 scratch. Nevertheless, depending on how different were the new ecosystem to
190 model, the require code changes could be quite significant.

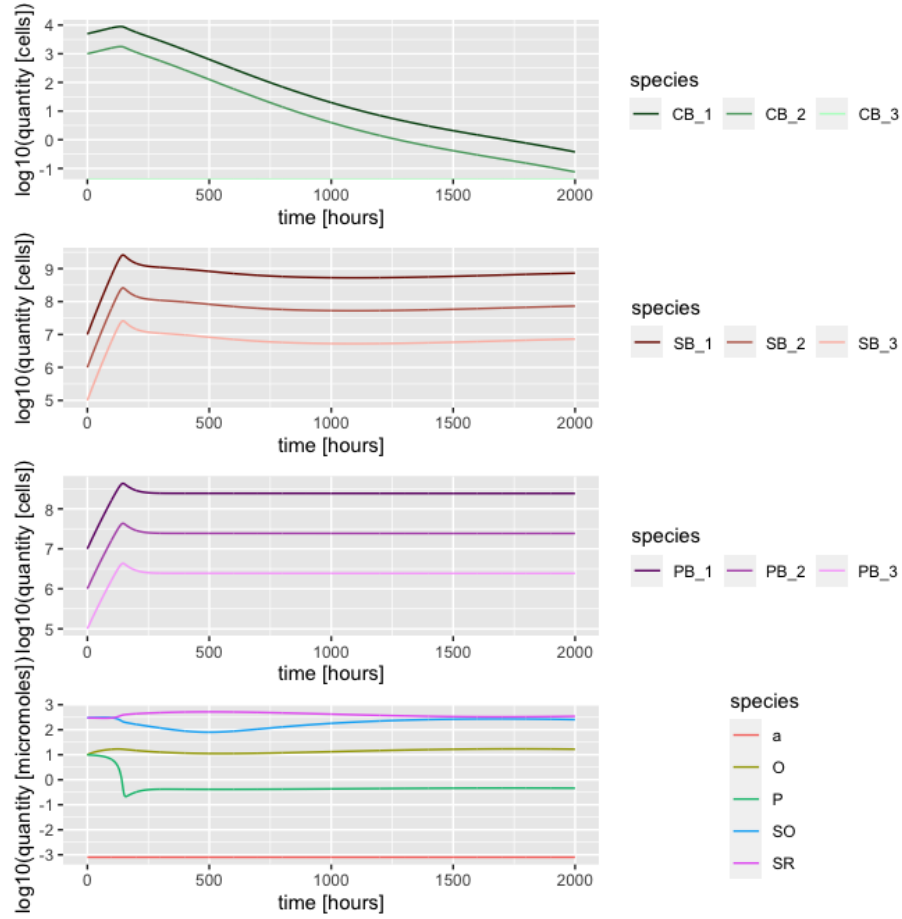


Figure 2: Plot of results of a simulation run using the function `plot_dynamics()`. Details can be found in the "User Guide" section "Three strains per functional group".

We evidence the impact of the *microxanox* package by describing three use cases, each of which was only possible with the package and that contains new results. The first two use cases are described in detail in the User Guide and the Partial Reproduction Vignettes. The third is taken from REF NEEDED [8] for which this R package was designed. All of these use cases can be expanded to larger numbers of strains per functional group and variable values can be changed.

5.1. Use case 1: Regime shifts during temporal environmental change

The package contains functionality to make a specific pattern of temporal change in the environmental condition oxygen diffusivity; this functionality forms the basis of the temporal method for finding stable states. A simple example of this functionality is given in the Partial Reproduction vignette, which we briefly show here (Figure @ref(fig:uc1)). The example is composed of a single simulation, at the beginning of which the system is in the oxic state with high abundance of cyanobacteria. Oxygen diffusivity is then slowly decreased and eventually, around hour 30'000 the system switches to the anoxic state, with high abundance of both sulfur bacteria types. The oxygen diffusivity is then quickly increased and at around hour 38'000 the system abruptly switches back to the oxic state.

5.2. Use case 2: The extent of hysteresis depends on community composition

The package also contains a function to extract summary features of ecosystem responses to environmental change, such as the amount of hysteresis displayed by the ecosystem. Hysteresis is a key feature of ecosystem responses to environmental change, because it is related to how difficult it can be to reverse the effects of environmental change [9]. The amount of hysteresis was measured here as the extent of the environmental condition for which there were two stable states. I.e. it was the extent of the environmental conditions for which historical conditions play an important role in determining the current system state (a definition of hysteresis). The results show that the amount of hysteresis depends greatly on the combinations of organisms present (Figure @ref(fig:uc2)). For example, with only the CB (cyanobacteria) present, there was no hysteresis. In contrast, the presence of both CB and SB (sulfate reducing bacteria) led to a large amount of hysteresis. (These results are also given in the Partial Reproduction vignette.)

?]... the figure needs beautifying please. ?]: is this OK like this?

5.3. Use case 3: Effects of functional diversity on regime shifts

As discussed in the Introduction section, the package was largely motivated by the question of how biodiversity influences ecosystem responses to environmental change. Extensive results concerning this question are given in a separate publication Limberger [5]. Here we describe one of the results, which is that having biodiversity in a functional group can allow state changes to occur that otherwise would not have. I.e. biodiversity can qualitatively change the state of the ecosystem.

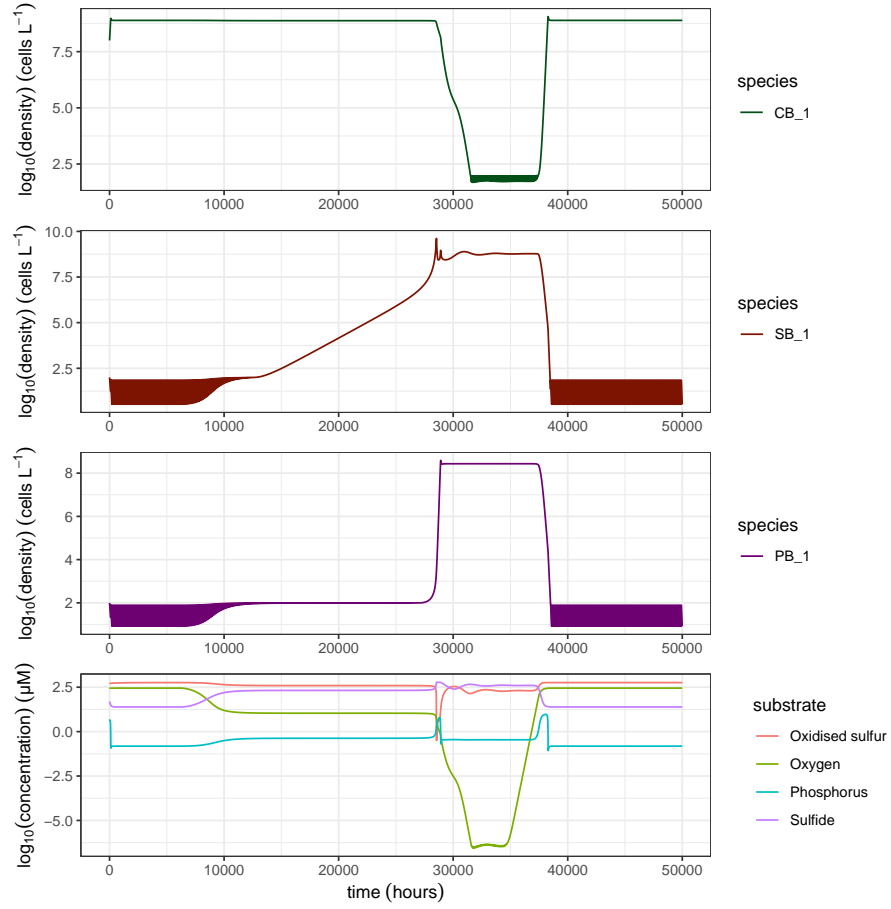


Figure 3: The temporal dynamics of the ecosystem model when an environmental condition (here parameter $*a*$, the oxygen diffusivity) changes. Plot of the stable states of the simulation runs under different oxygen diffusivity.

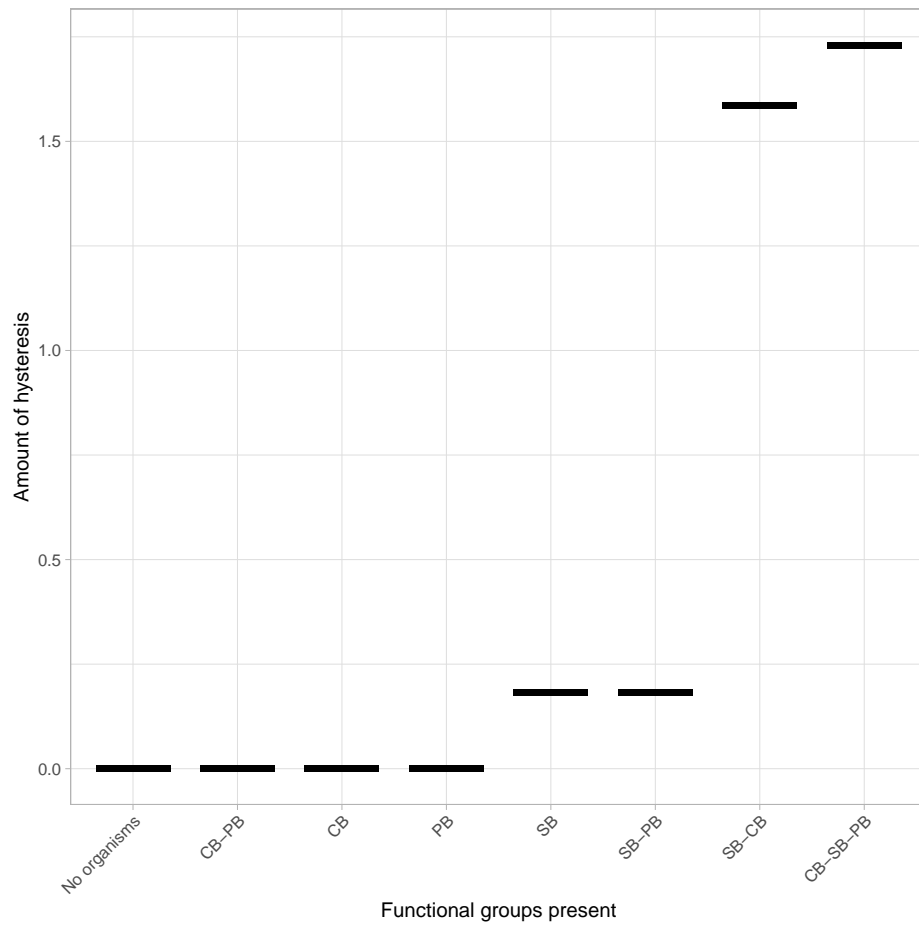


Figure 4: The amount of hysteresis depends on the combination of types of organisms present.

Biodiversity was added to the functional groups using the `new_strain_parameter()` function to create a parameter set with multiple species per functional group (albeit all with identical features) and then to add variability among the species by calling the `add_strain_var()` function. This function takes an already existing parameter set and adds the specified amount of variation. The new parameter object is then used as before.

Figure @ref(fig:uc3) shows a simulation with two species (strains) in each of the three functional groups. The ecosystem starts in the oxic state, though with relatively high abundance of each functional group. The strain of SB that is more tolerant to oxygen (SB_1) initially decreases in abundance, but then increases, and the other (SB_2) strain then becomes abundant and SB_1 declines. Furthermore, the cyanobacteria crash in abundance, and the system switches to the anoxic state. Importantly, the switch does not occur if there are two identical strains with tolerance half way between those in Figure @ref(fig:uc3).

Rainer... please beautify the figure as required. It comes from the Limberger et al supplement, Figure 5.4 ?]: is this OK like this? Used the graph from the supplement

251 6. Conclusions

{»Set out the conclusion of this original software publication.«}

microxanox allows the simulation, visualisation, and analysis of a model of a microbial ecosystem while allowing variation in the amount of diversity contained in each of the functional groups of organisms present. It has been used for the research described in another paper of ours that is one of the first investigations of the effects of diversity on ecosystem resilience Limberger [5]. In that paper, we show that diversity can have large and important effects of ecosystem responses, highlighting the need for models such as ours, within which one can easily manipulate the amount of biodiversity. The *microxanox* package has also been used to reproduce the results of the paper that inspired the package development Bush et al. [2].

The package greatly lowers the amount of work required in further investigations of the specific ecosystem modelled. There has, for example, been quite limited investigation of how biodiversity influences the short-term responses of the modelled ecosystem to environmental change. Likewise, the package could be used to power an investigation of the effects of biodiversity on the usefulness of early warning signals of abrupt ecosystem change [10]. In addition this package could be used as a template for the implementation for developing models of other types of ecosystems and organism. By doing so, other models can profit from the overall framework used, and the reproducibility aspects as well as the flexibility implemented.

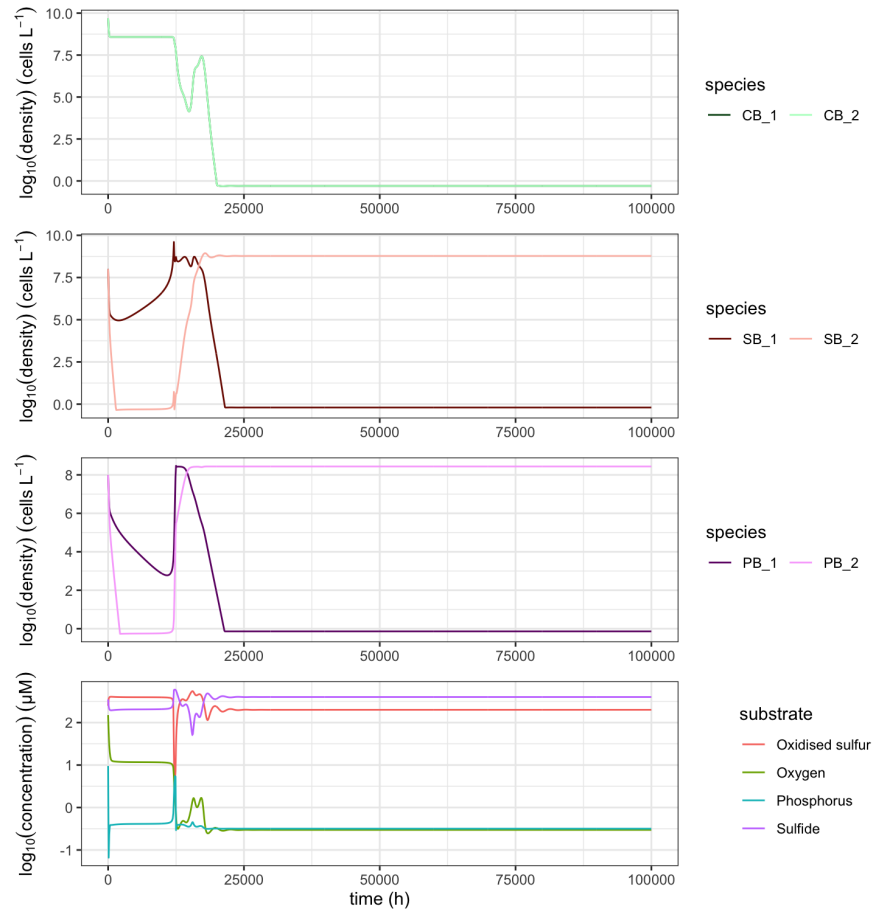


Figure 5: The dynamics of the ecosystem when there are two species in each functional group, and some variation (diversity) in species parameters.

273 7. Conflict of Interest

274 The authors declare no known conflicting or competing interests associated
275 with this publication and there has been no significant financial support for this
276 work that could have influenced its outcome.

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