R package rodeoFABM: Basic Use and Sample Applications

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Contents

1 Main features of `rodeoFABM`

The `R` package `rodeoFABM` is a colletion of functions to help create water quality models that can be coupled to physical host models using the `FABM` interface (Bruggeman and Bolding (2014)). As the name suggests it is heavily influenced by the `R` package `rodeo` (Kneis, Petzoldt, and Berendonk (2017)). The principle idea is to provide functions that:

- Decouple the "code writing" from the "model development" part of creating a model
- Make model adaptation, communication, and maintenance easier

The main concept is to write down the model equations in the standard Peterson matrix notation and store them in text files or spread sheets. The package `rodeoFABM` then can be used to automatically generate `FABM` specific FORTRAN code from these files, create `.yaml` control files for the water quality model and generate LaTeX documentation of the model. For some operating systems there are also functions to automatically compile the 1D physical lake model `GOTM` (Burchard et al. (2006)) coupled with the model. The package also containse some functions to read into R and plot the outcome of a coupled `GOTM-FBAM` model run.

2 Installation and requirements

So far `rodeoFABM` was only tested with different Linux based operating systems, but besides compiling `GOTM-FABM` the contained funcitons should run on all operating systems. To create the `FABM` specific source code only some other R packages are required:

- `readODS`
- `plot3D`
- `ncdf4`
- `reshape2`
- `RColorBrewer`

In order to automatically compile `GOTM-FABM` and run the examples in this vignette some additional software tools are needed:

- The GNU compilers (gcc.gnu.org)
- GNU Make (gnu.org/software/make/)
- GNU CMake (cmake.org)
- git (git-scm.com)
- the netcdf libraries

The package `rodeoFABM` can be installed from github using:

```
library("devtools")
install_github("JFeldbauer/rodeoFABM")
```

3 Basic use

3.1 First example

To demonstrate the work flow we will create and compile a simple model. The files used in this example are contained in the package and can be copied to the current working directory using:

```
# copy example ods file
example_model <- system.file("extdata/simple_model.ods", package = "rodeoFABM")
file.copy(from = example_model, to = ".", recursive = TRUE)
```

This will copy the Libre Office spread sheet *simple_model.ods* to your current working directory. Now we can read in the tables with the declarations of state variables, model parameters, used functions and external dependencies, process rate descriptions, and stoichiometry matrix.

```
library(readODS)

# read in example ods file
odf_file <- "simple_model.ods"
vars <- read_ods(odf_file, sheet = 1)
pars <- read_ods(odf_file, sheet = 2)
funs <- read_ods(odf_file, sheet = 3)
pros <- read_ods(odf_file, sheet = 4)
stoi <- read_ods(odf_file, sheet = 5)
```

We store the declarations in the five data frames *vars*, *pars*, *funs*, *pros*, and *stoi*. Using these we can now generate FORTRAN source files using the function `gen_fabm_code()`

```
library(rodeoFABM)

# generate fabm code
gen_fabm_code(vars,pars,funs,pros,stoi,"simple_model.f90",diags = TRUE)
```

This will create two new files: the *FABM* specific FORTRAN source code *simple_model.f90* and the control file *fabm.yaml* which can be used to change model parameters and initial conditions. The function also checks if all parameter, functions, and state variables used are also decalred and issues a warning because the units decalred for the parameters are not in seconds, which is required by *FABM*.

Using the source code file *simple_model.f90* we can compile *GOTM-FABM*. Therfore we first need to clone the lake branche of *GOTM* from github and prepare the build process. This can automatically be done using the function `clone_GOTM()`:

```
# clone github repo
clone_GOTM(build_dir = "build", src_dir = "gotm_src")
```

This will take a moment and download the source code for *GOTM* and *FABM* as well as prepare the compilation using *CMake*. You can see that there are now two new folders in the working directory called *gotm_src* and *build*. Now we can build *GOTM-FABM* with our simple model using the *simple_model.f90* file and the `build_gotm()` function:

```
# build GOTM
build_GOTM(build_dir = "build",fabm_file = "simple_model.f90",
           src_dir = "gotm_src")
```

This will copy the *simple_model.f90* file we just created to the correct folder within the *gotm_src* folder and then compile *GOMT-FABM* using *make*. As a last step it will copy the created executable to the current working directory. You can see that there is now a *gotm* executable file in the working directory. In order to run our created model we will need a *gotm.yaml* file (the GOTM controll fille), an hypsograph file, and the meteorological forcing data. We will copy the example files provides in this package by using:

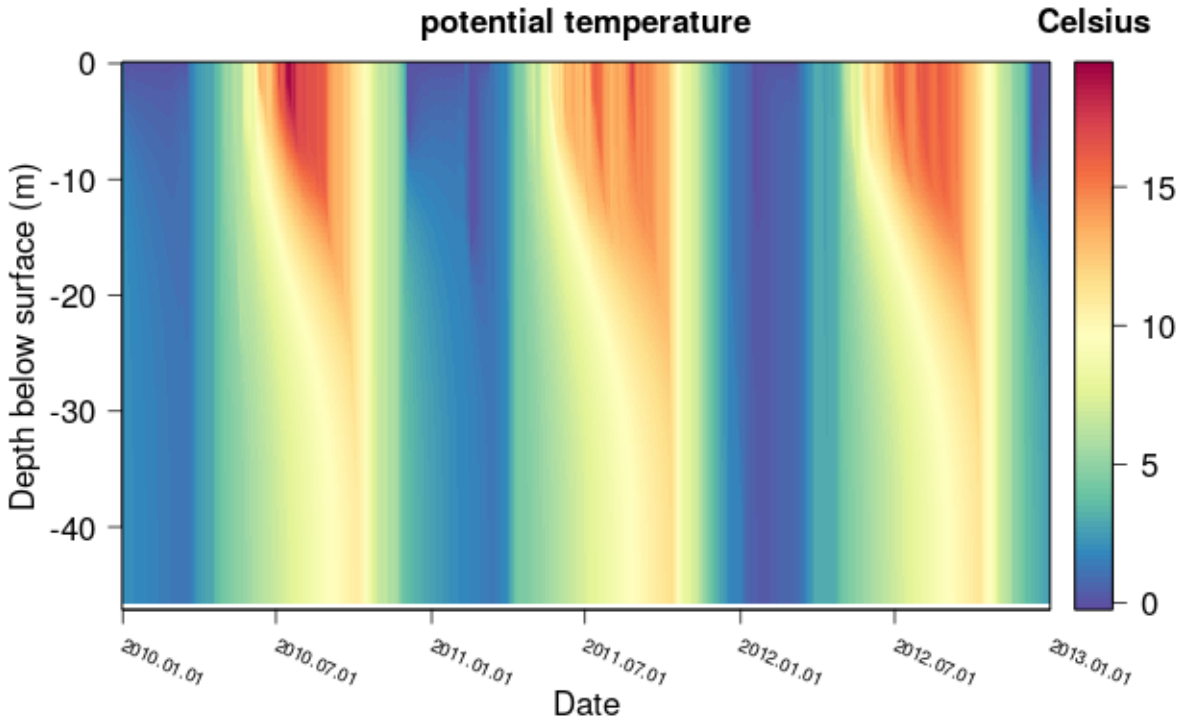
```
# copy example gotm.yaml
yaml <- system.file("extdata/gotm.yaml", package = "rodeoFABM")
file.copy(from = yaml, to = ".", recursive = TRUE)
# write hypsograph
write.table(hypsograph, "hypsograph.dat", sep = "\t", row.names = FALSE,
            quote = FALSE)
# write meteo data
write.table(meteo_file, "meteo_file.dat", sep = "\t", row.names = FALSE,
            quote = FALSE)
```

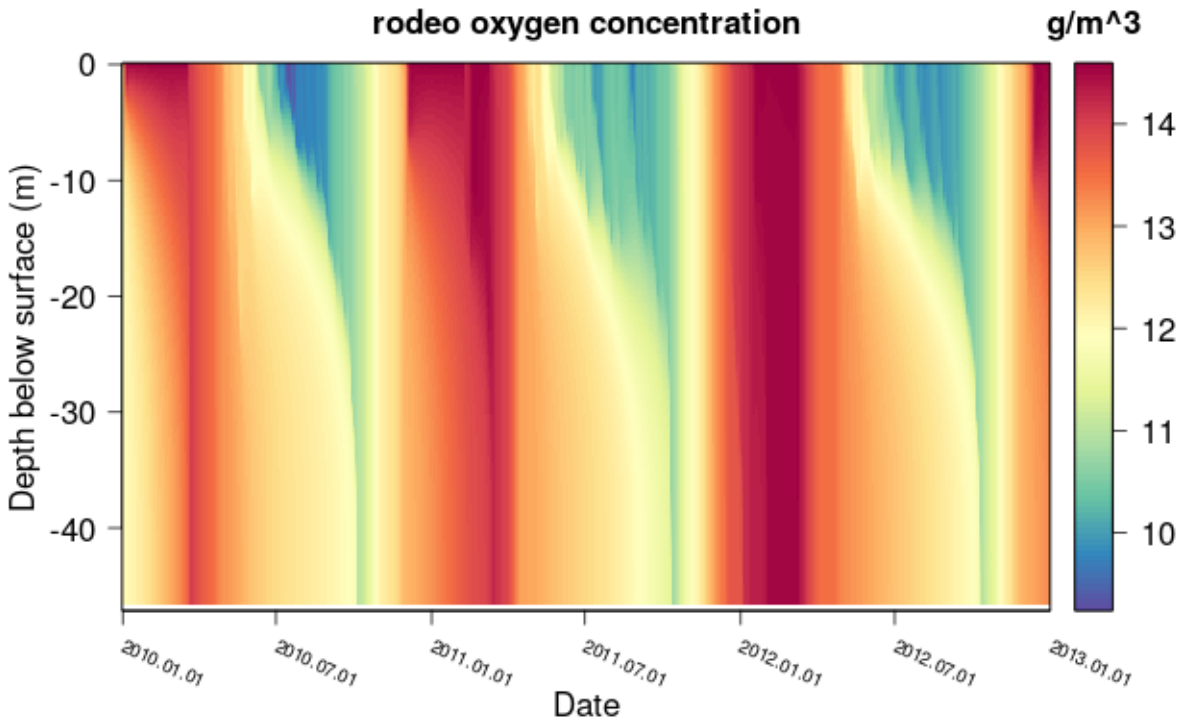
Now that we have the files *gotm.yaml*, *hypsograph.dat*, and *meteo_file.dat* in our working directory, we can run *GOTM-FABM* using:

```
# run gotm
system2("./gotm")
```

After successfully running there are two new files: *output.nc* and *restart.nc*, both are netcdf files. *output.nc* is the output of the model run and *restart.nc* is a netcdf file that can be used to initialize a simulation with states stored from the previous run. We can plot the results e.g. by using the `plot_var()` function:

```
# plot temperature
plot_var("output.nc", "temp")

# plot oxygen
plot_var("output.nc", "rodeo_C_O2")
```





These are the essential steps used to build and run a *GOTM-FABM* model. In the next section we will go a little bit more into the details of building a own model using the `rodeoFABM` package and explain them step by step.

3.2 Manually compiling GOTM-FABM

If the provided compilation functions do not work on your operating system instructions on how to include your newly created FABM model can be found in the FABM wiki: github.com/fabm-model/fabm/wiki/Developing-a-new-biogeochemical-model. Instructions on how to compile GOTM-FABM can be obtained from the GOTM homepage: gotm.net/portfolio/software/.

3.3 Create a model step by step

In order to demonstrate the necessary steps and functionalities we will create a simple phytoplankton-nutrients model and progressively add more processes and state variables.

All used Libre Office spread sheets containing the model information, the GOTM control file, and the forcing data are contained in the rodeoFABM package. You can copy all necessary files to run GOTM using the same method as described in the first example. We will use the same meteorological forcing (*meteo_file.dat*) and hypsographic curve (*hypsograph.dat*) as in the first example. Additionally we now add one inflow and one outflow (files inflow_m.dat, outflow.dat, and inflow_wq_m.dat containing the nutrient concentrations of the inflow)

```
## copy necessary files

# GOTM controll fille
yaml <- system.file("extdata/examples/gotm.yaml",
                    package = "rodeoFABM")
file.copy(from = yaml, to = ".", recursive = TRUE)
# inflow hydrological data
infl <- system.file("extdata/examples/inflow_m.dat",
                    package = "rodeoFABM")
file.copy(from = infl, to = ".", recursive = TRUE)
# inflow nutient data
nut <- system.file("extdata/examples/inflow_wq_m.dat",
                    package = "rodeoFABM")
file.copy(from = nut, to = ".", recursive = TRUE)
# outflow data
out <- system.file("extdata/examples/outflow.dat",
                    package = "rodeoFABM")
file.copy(from = out, to = ".", recursive = TRUE)
```

The inflows and especially the inflow of state variables to a *FABM* model are defined in the streams section of the *GOTM* control file (*gotm.yaml*). The section looks like this:

```
streams:
   inflow:                                  # stream configuration
      method: 4                               # inflow method, default=1
      zu: 0.0                                 # upper limit m
      zl: 0.0                                 # lower limit m
      flow:                                   # water flow
         method: 2                            # 0=constant, 2=from file, default = 0
         constant_value: 1.0                  # constant value( m^3/s)
         file: inflow_m.dat                   # path to file with time series
         column: 1                            # index of column to read from
      temp:                                   # flow temperature
         method: 2                            # 0=constant, 2=from file; default=0
         constant_value: 10.0                 # constant value (°C)
         file: inflow_m.dat                   # path to file with time series
         column: 2                            # index of column to read from
```

```
      salt:                                    # flow salinity
         method: 0                             # 0=constant, 2=from file; default=0
         constant_value: -1.0                  # constant value (PSU)
         file: inflow.dat                      # path to file with time series
         column: 3                             # index of column to read from
      rodeo_HPO4:                              # rodeo phosphprus
         method: 0                             # 0=constant, 2=from file; default=0
         constant_value: 0.5                   # constant value (gP/m^3)
         file: inflow_wq_m.dat                 # path to file with time series
         column: 4                             # index of column to read from
```

Within the `streams` section several in- and outflows can be defined with any desired name (here "inflow"). The inflow/outflow depth is defined by `streams/method`, whereas `1` means surface, `2` means bottom, `3` means a specified range of depths defined by `streams/zu` (upper) and `streams/zl` (l), and `4` means inflow to the depth with same temperature as the inflow temperature. Every in- or outflow needs the `streams/flow` section defining the flow rate in m^3/s and can have additional entries like `streams/temp` for temperature or inflowing state variables of the *FABM* model (like `streams/rodeo_HPO4`). The *FABM* sate variables need to start with *rodeo_* followd by the defined state variable name. The values can either be constant (`streams/rodeo_HPO4/method` = 0) or a time series given by a tab separated file (`streams/rodeo_HPO4/method` = 2) with first column datetime (as `YYYY-mm-dd HH:MM:ss`). The name of the file is supplied by `streams/rodeo_HPO4/file` and the column the variable is in by `streams/rodeo_HPO4/column`, take care: the first column with datetime is not counted and if the columns have a header it needs to start with an excalamation mark "!".

We can create the source code of the phytoplankton nutients model in the same way as we created the source code in the first example:

```
# copy the spread sheet
ods <- system.file("extdata/examples/simple_alg.ods",
                   package = "rodeoFABM")
file.copy(from = ods, to = ".", recursive = TRUE)

# declare data frames for vars, pars, funs, pros, and stoi
vars <- read_ods("simple_alg.ods", sheet = "vars")
pars <- read_ods("simple_alg.ods", sheet = "pars")
funs <- NULL
pros <- read_ods("simple_alg.ods", sheet = "pros")
stoi <- read_ods("simple_alg.ods", sheet = "stoi")
```

This first model is a simple model with two state variables, which are declared in the `vars` data frame. The table needs to have at least three columns: *name* giving the identifier of the state variable, *unit* giving the used unit, and *description* giving a short description of the state variable. If additionally the column *default* is supplied the initial value will be included in the *FABM* control file (`fabm.yaml`), which is automatically generated by `gen_fabm_code()`.

Table 1: Data frame `vars`: Declaration of state variables.

name	unit	description	default
C	gDM/mˆ3	algae concentration	0.0
$HPO4$	gP/mˆ3	phosphorus concentration	0.1

The models parameters are defined in the `pars` data frame in a similar fashion. They need the same three columns *name*, *unit*, and *description* and can have the aditional column *default* as well. Take care that *FABM* requires all parameters with relation to time to be in units of second.

Table 2: Data frame `pars`: Declaration of model parameters.

name	unit	description	default
mu_max	1/s	maximum growth rate	1e-05
K_P	W/m^2	half saturation concentration of HPO4 limitation	2e-02
k_death	1/s	death rate	2e-06
a_P	gP/gDM	phosphorus content of phytoplankton	5e-02

External functions, or forcing data that needs to be obtained from the physical host model (e.g. water temperature) are defined in `funs`. As this first model has no such functions or dependencies this is explaine in the later steps. As in this example the data frame is not needed it hast to be set to `NULL`.

The declaration of the processes and process rates is done in the `pros` data frame. It has four requred columns: *name* giving the name of the proicess, *unit* giving the unit of the process rate (again in seconds), *description* giving a short description of the process, and *expression* giving the mathematical expression of the process. There can be additional columns to define the saptial domain of the process, or to declare sinking processes and they will be explained later.

Table 3: Data frame `pros`: Declaration of processes.

name	unit	description	expression
growth	g/m^3/d	growth of algae	$C \cdot mu\_max \cdot HPO4/(HPO4 + K\_P)$
death	g/m^3/d	death of algae	$C \cdot k\_death$

In this model the phytoplankton have a simple linear growth term with a Monod like limitation for the limiting nutrient Phosphorus and a linear decay/death term.

The last data frame `stoi` gives the stoichiometry table (in long format) connecting the process rates with the state variables. It has three required columns: *variable* giving the variable affected by the *process*, and *expression* giving a factor to multiply the process rate by:

Table 4: Data frame `stoi`: Declaration of stoichiometry matrix in long format.

variable	process	expression
C	growth	1
C	death	-1
$HPO4$	growth	$-1 \cdot a\_P$

The growth of phytoplankton is increasing its concentration C and decreasing the nutrient $HPO4$ by the fraction of a_P, which is the Phosphorus conten of the phytoplankton. Decay/death is decreasing phytoplankton concentration C.

Having declared all five data frames we can now generate the fortran code using `gen_fabm_code()`. This will also perfome some automated checks e.g. if all used parameters and state variables are also declared, and will issue a warning if the used units are not using seconds for time. It will also create the *FABM* control file `fabm.yaml` and insert the default values for parameters and initial values (if declared). If the argument `diags` is set to TRUE the process rates are stored as diagnostic variables in the output netcdf file.

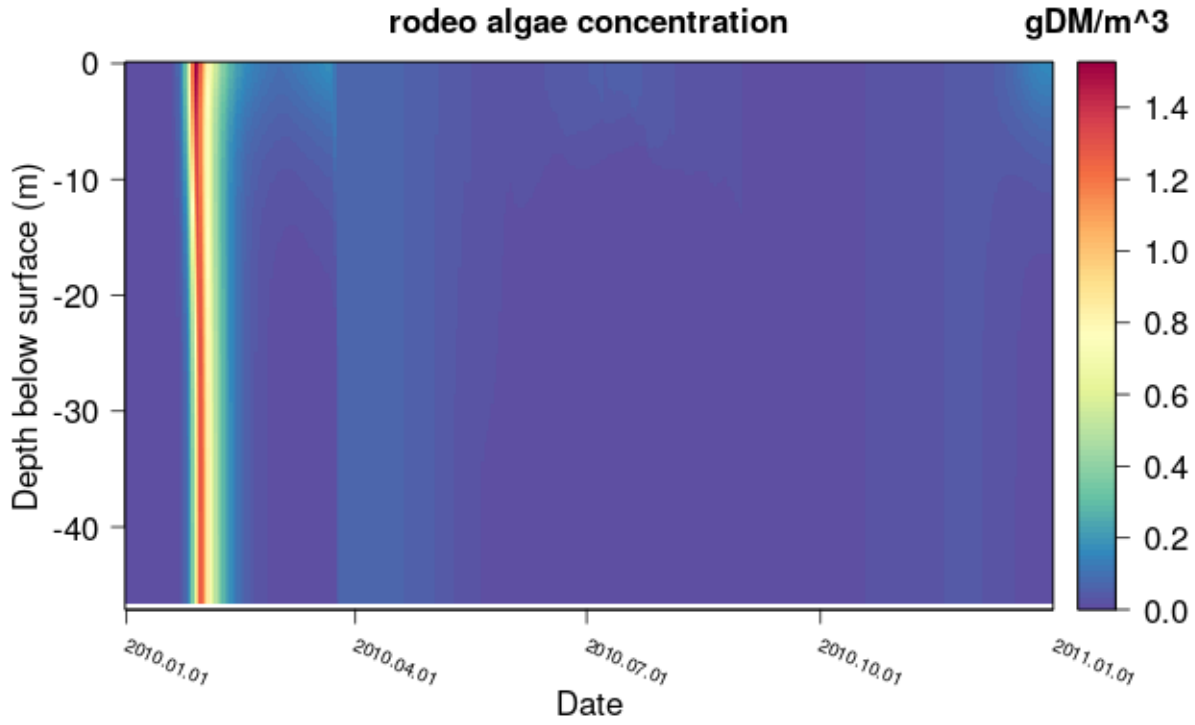
```
# create the fabm code
gen_fabm_code(vars, pars, funs, pros, stoi, "model_1.f90", diags = TRUE)
```

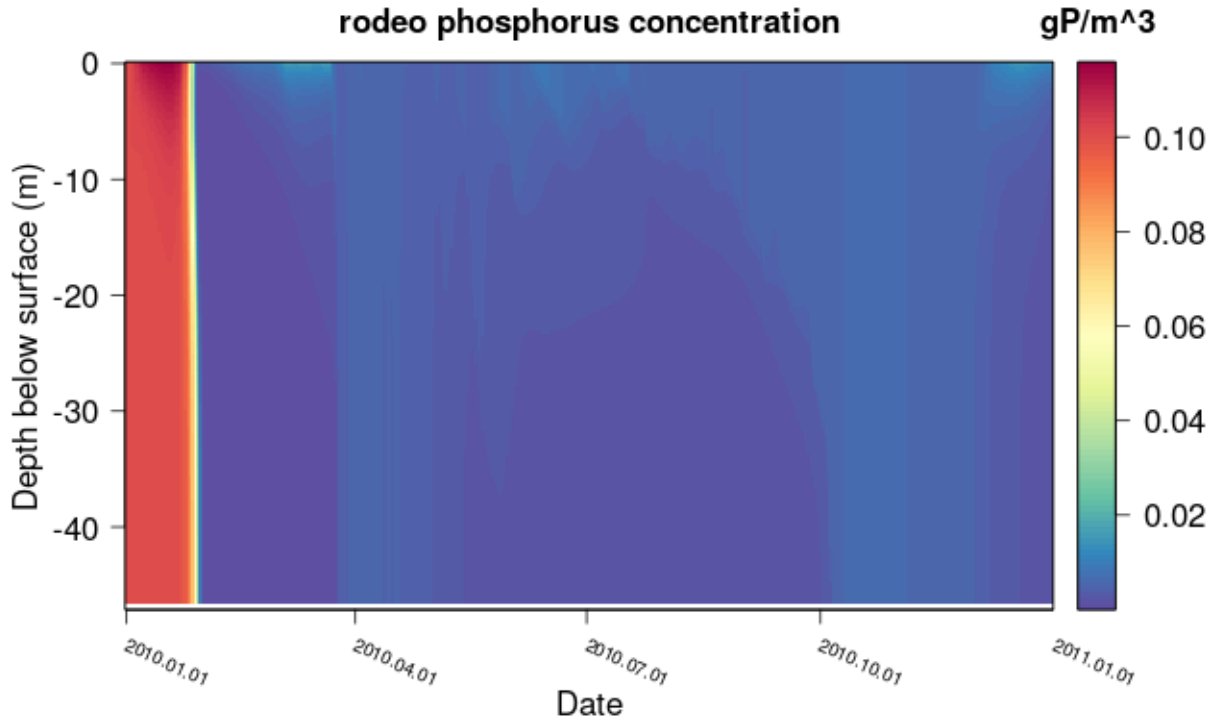
After creating the fortran source code, *GOTM-FABM* can be automatically compiled unsing the function `build_GOTM()` (assuming the source code was allready fetched and prepared for compilation using `clone_GOTM()`), this will also copy the compiled executable to the current working directory, which then can be ran using e.g. `system2("./gotm")`.

```
# build GOTM with the model
build_GOTM(build_dir = "build", src_dir = "gotm_src",
           fabm_file = "model_1.f90")

# run the model
system2("./gotm")
```

We can now plot the model results e.g. using the `plot_var()` function:

```
# plot the variables
plot_var("output.nc", "rodeo_C")
plot_var("output.nc", "rodeo_HPO4")
```





3.3.1 Getting dependencies from the host model

As many biogeochemical processes depend on external forcing, such as temperature or available iradiation, these values can be obtained from the physical host model. In the next step we want to add the dependency of phytoplankton growth on available iradiation. We first copy the prepared spread sheet and declare the data frames:

```
ods <- system.file("extdata/examples/simple_alg_par.ods",
                   package = "rodeoFABM")
file.copy(from = ods, to = ".", recursive = TRUE)

# declare data frames for vars, pars, funs, pros, and stoi
vars <- read_ods("simple_alg_par.ods", sheet = "vars")
pars <- read_ods("simple_alg_par.ods", sheet = "pars")
funs <- read_ods("simple_alg_par.ods", sheet = "funs")
pros <- read_ods("simple_alg_par.ods", sheet = "pros")
stoi <- read_ods("simple_alg_par.ods", sheet = "stoi")
```

We need to get values for the photosynthetic active radiation (PAR) from GOTM. *FABM* has so called "standard-variables" with defined names (stored in the `std_names_FABM` data). If you want to access these variables you need to defind them as a function in the `funs` data frame and add the additional column *dependency* wich contains the full standard-variable name. The data frame `funs` has three required columns that are the same as in `vars`, and `pars`: *name*, *unit*, and *description*, additionally the column *dependency*. If you declare several functions of whome some are not dependencies the corresponding entry in column *dependency* needs to be empty (`NA`) for these and the corresponding standard-name for the ones that are dependencies.

Table 5: Data frame `funs`: Declaration of model functions and dependencies from the host model.

name	unit	description	dependency
par	W/m^2	Downwelling photosynthetic radiative flux	downwelling_photosynthetic_radiative_flux

The declared functions/dependencies can now be used in the process expression, same as parameters and state variables. We added a Monod Term for light limitation in the *growth* process:

Table 6: Data frame `pros`: Declaration of processes.

name	unit	description	expression
growth	g/m^3/d	growth of algae	$C \cdot mu\_max \cdot HPO4/(HPO4 + K\_P) \cdot par/(par + K\_par)$
death	g/m^3/d	death of algae	$C \cdot k\_death$

For this we need to declare the additional parameter *K_par* for the half-saturation irradiation in the `pars` data frame:

Table 7: Data frame `pars`: Declaration of model parameters.

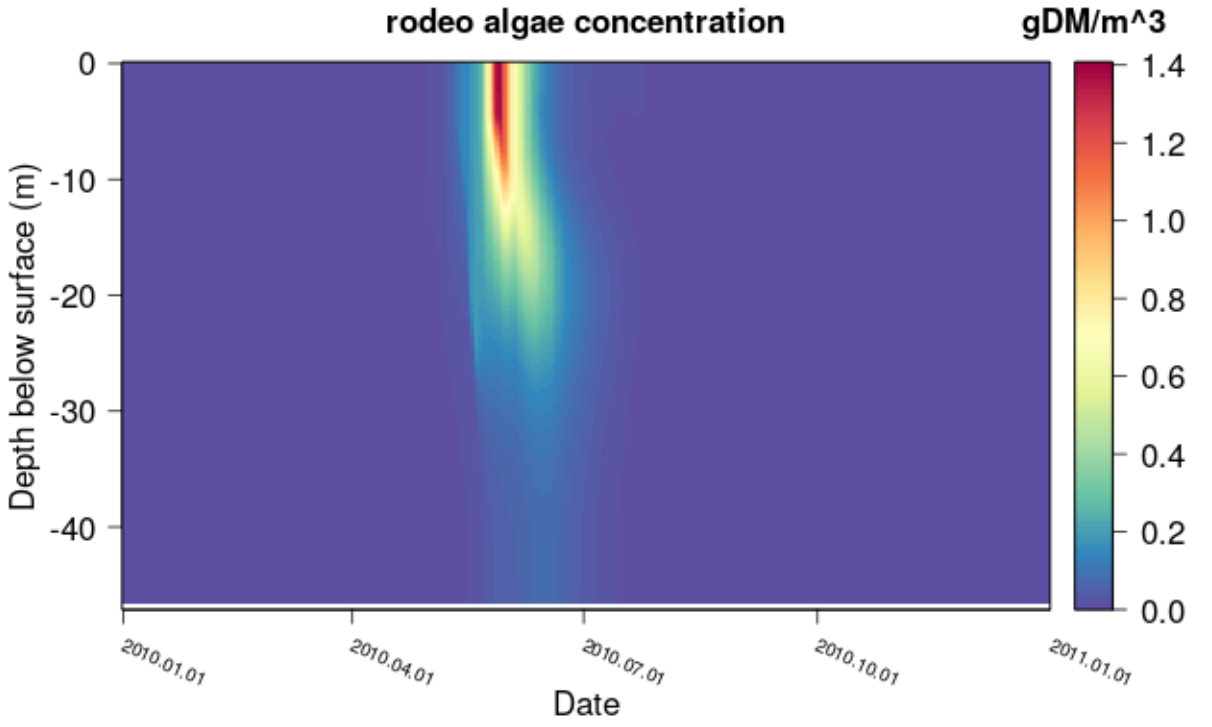
name	unit	description	default
mu_max	1/s	maximum growth rate	1.0e-05
K_P	W/m^2	half saturation of photosyntetic flux	2.0e-02
k_death	1/s	death rate	2.0e-06
a_P	gP/gDM	phosphorus content of phytoplankton	5.0e-02
K_par	W/m^2	half saturation of photosyntetic flux	2.7e+01

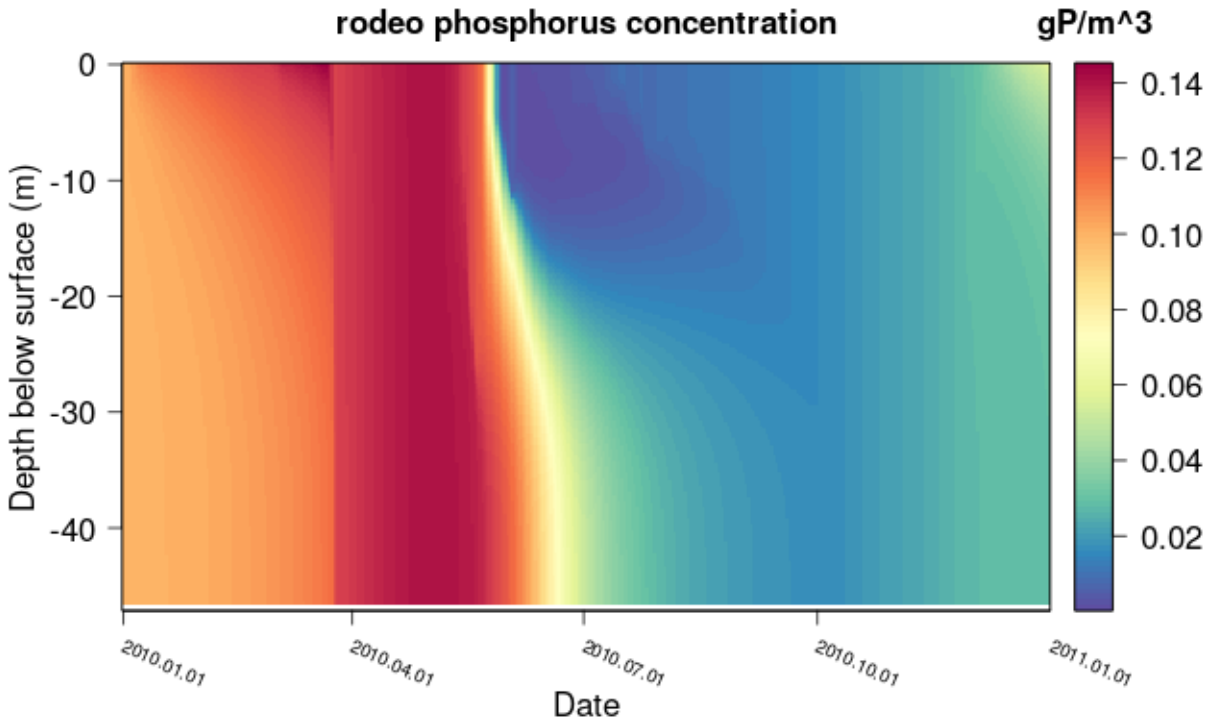
Now we can generate the fortran code, compile *GOTM-FABM*, and run the adapted model.

```
# create the fabm code
gen_fabm_code(vars, pars, funs, pros, stoi, "model_2.f90", diags = TRUE)

# build GOTM with the model
build_GOTM(build_dir = "build", src_dir = "gotm_src",
           fabm_file = "model_2.f90")

# run the model
system2("./gotm")
```

And plot some of the simulated state variables:

```
# plot the variables
plot_var("output.nc", "rodeo_C")
plot_var("output.nc", "rodeo_HPO4")
```

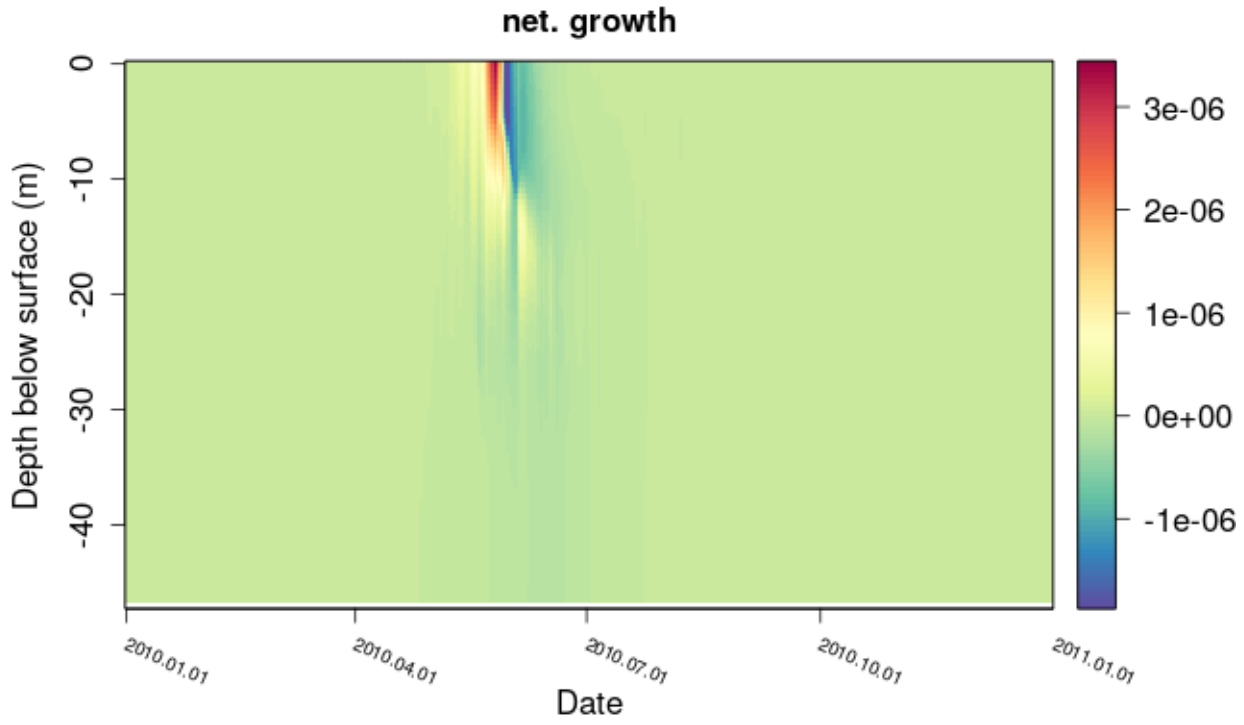




From the saved process rates (the diagnostic variables) we can e.g. plot the net growth rate. We can acces the values stored in the netcdf file e.g. by using the function `get_var()` and plot them using `plot3D::image2D()`:

```
library(plot3D)
```

```
# also plot net. growth
growth <- get_var("output.nc", "rodeo_growth")
death <- get_var("output.nc", "rodeo_death")
net_growth <- growth$var - death$var
# nice colors
mycol <- colorRampPalette(rev(RColorBrewer::brewer.pal(11, 'Spectral')))
# plot the net. growth
image2D(net_growth, growth$time, growth$z, main = "net. growth", col = mycol(100), xaxt = "n",
        xlab = "Date", ylab = "Depth below surface (m)")
axis(1, at = pretty(growth$time), labels = FALSE)
text(pretty(growth$time), par("usr")[3] - 3, labels = format(pretty(growth$time), "%Y.%m.%d"),
     xpd = NA, srt = 336, adj = 0.0, cex = 0.8)
```



3.3.2 Sedimentation

Often in biogeochemical models some state variables are sinking in the water body (e.g. phytoplankton or particulated organic matter). In the next adaptation of the model we want to include a constant sinking velocity for the phytoplankton. Therefore, we again copy the spread sheets from the package data in order to declare the data frames:

```
ods <- system.file("extdata/examples/simple_alg_par_sed.ods",
                   package = "rodeoFABM")
file.copy(from = ods, to = ".", recursive = TRUE)

# declare data frames for vars, pars, funs, pros, and stoi
vars <- read_ods("simple_alg_par_sed.ods", sheet = "vars")
pars <- read_ods("simple_alg_par_sed.ods", sheet = "pars")
funs <- read_ods("simple_alg_par_sed.ods", sheet = "funs")
pros <- read_ods("simple_alg_par_sed.ods", sheet = "pros")
```

```
stoi <- read_ods("simple_alg_par_sed.ods", sheet = "stoi")
```

FABM allows for time varying sinking of state variables. This in implemented in *rodeoFABM* as a process declared in the `pros` data frame that has a logical flag set in an additional column called *sedi*. The expression for this can also be a function of external dependencies (e.g. water density) or internal state variables (e.g. nutrient concentration), in this simple case we choose a constant sinking velocity:

Table 8: Data frame `pros`: Declaration of processes.

name	unit	description	expression	sedi
growth	g/m^3/d	growth of algae	$C \cdot mu\_max \cdot HPO4/(HPO4 + K\_P) \cdot par/(par + K\_par)$	NA
death	g/m^3/d	death of algae	$C \cdot k\_death$	NA
sed	g/m^3/s	sinking	v_sed	TRUE

For this to work we need to declare the additional parameter for the sinking velocity:

Table 9: Data frame `pars`: Declaration of model parameters.

name	unit	description	default
mu_max	1/s	maximum growth rate	1.0e-05
K_P	W/m^2	half saturation of photosyntetic flux	2.0e-02
k_death	1/s	death rate	2.0e-06
a_P	gP/gDM	phosphorus content of phytoplankton	5.0e-02
K_par	W/m^2	half saturation of photosyntetic flux	2.7e+01
v_sed	m/s	sedimentation velocity	1.0e-06

And add the process to the stopichiometry table:

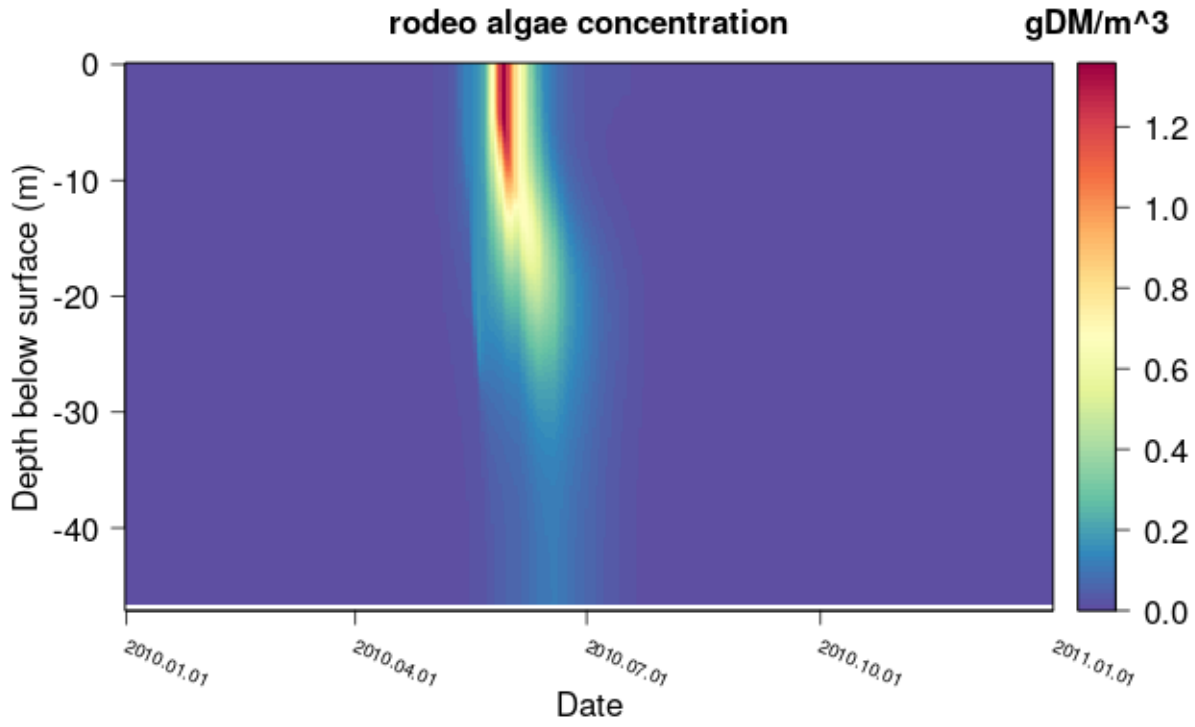
Table 10: Data frame `stoi`: Declaration of stoichiometry matrix in long format.

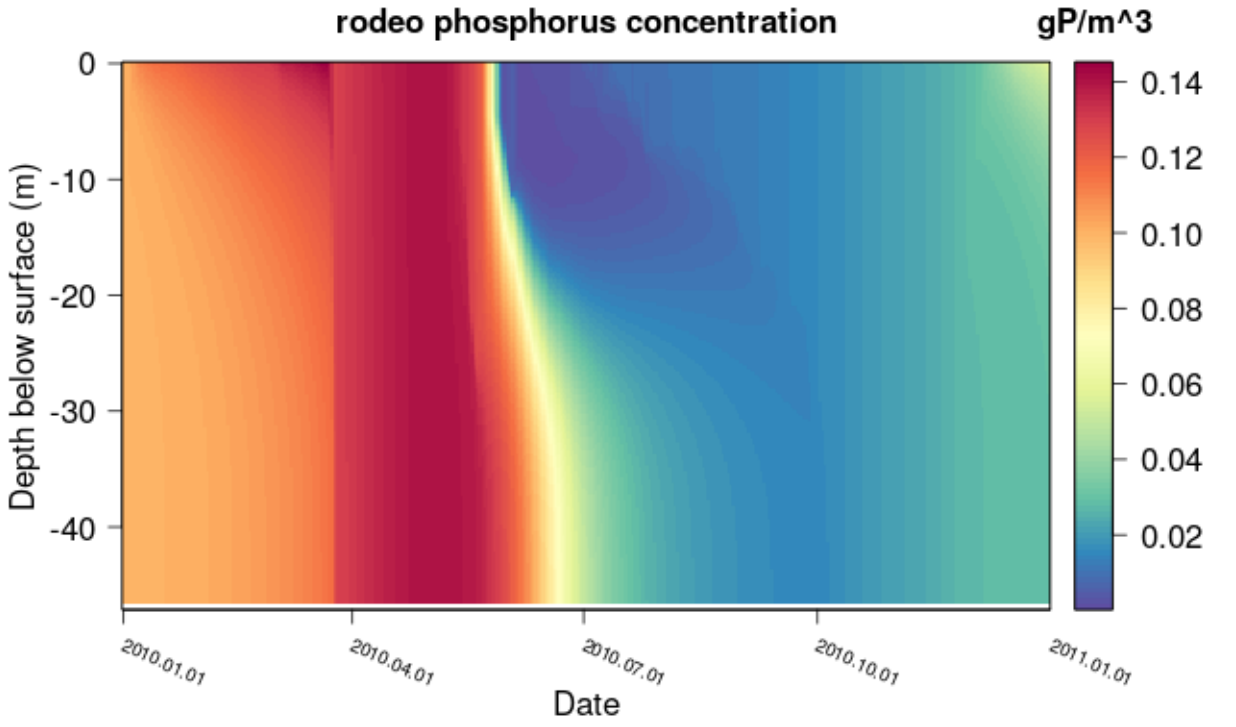
variable	process	expression
C	growth	1
C	death	-1
C	sed	-1
$HPO4$	growth	$-1 \cdot a\_P$

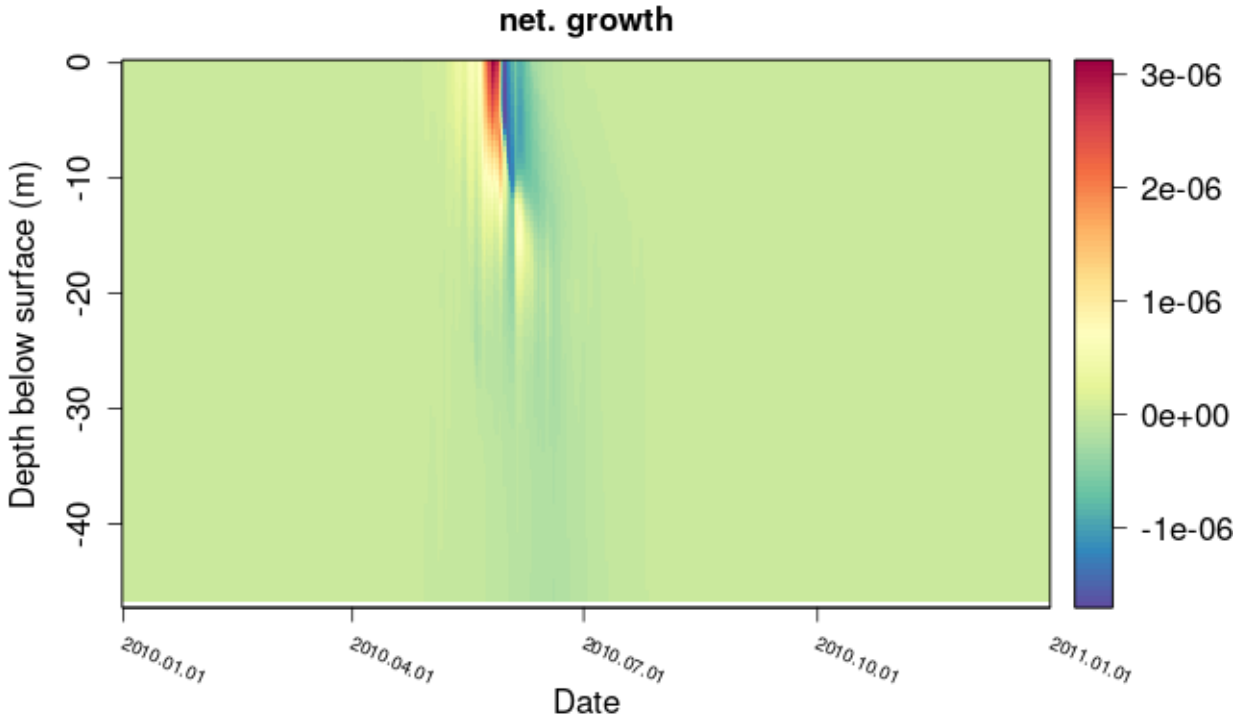
Now we can create the FORTRAN source code file, compile *GOTM-FABM*, run the model, and plot some of the results:

```
# create the fabm code
gen_fabm_code(vars, pars, funs, pros, stoi, "model_3.f90")

# build GOTM with the model
build_GOTM(build_dir = "build", src_dir = "gotm_src",
           fabm_file = "model_3.f90")

# run the model
system2("./gotm")
```

```r
# plot the variables
plot_var("output.nc", "rodeo_C")
plot_var("output.nc", "rodeo_HPO4")

# also plot net. growth
growth <- get_var("output.nc", "rodeo_growth")
death <- get_var("output.nc", "rodeo_death")
net_growth <- growth$var - death$var

image2D(net_growth, growth$time, growth$z, main = "net. growth", col = mycol(100), xaxt = "n",
        xlab = "Date", ylab = "Depth below surface (m)")
axis(1, at = pretty(growth$time), labels = FALSE)
text(pretty(growth$time), par("usr")[3] - 3, labels = format(pretty(growth$time), "%Y.%m.%d"),
     xpd = NA, srt = 336, adj = 0.0, cex = 0.8)
```







3.3.3 Processes at the surface and sediment

There are some processes that only take place at the surface or bottom (sediment) of lakes. *FABM* knows three spatial domains: open water (pelagial), surface, and bottom (sediment) and processes can be declared

to only take place at one of these domaines. To demonstrate this we add the new state variable Oxygen along with the processes of surface exchange and a constant oxygen consumption in the sediment to the model. We again start by copying the spread sheet from the package data:

```
ods <- system.file("extdata/examples/simple_alg_O2.ods",
                   package = "rodeoFABM")
file.copy(from = ods, to = ".", recursive = TRUE)
# read in first simple model
vars <- read_ods("simple_alg_O2.ods", sheet = "vars")
pars <- read_ods("simple_alg_O2.ods", sheet = "pars")
funs <- read_ods("simple_alg_O2.ods", sheet = "funs")
pros <- read_ods("simple_alg_O2.ods", sheet = "pros")
stoi <- read_ods("simple_alg_O2.ods", sheet = "stoi")
```

Here we added the new state variable $O2$ to the `vars` data frame:

Table 11: Data frame `vars`: Declaration of state variables.

name	unit	description	default
C	gDM/m^3	algae concentration	0.0
$HPO4$	gP/m^3	phosphorus concentration	0.1
$O2$	gO/m^3	oxygen concentration	10.0

If processes occure only at the surface or bottom interface we can declare this by setting a logical flag in additional columns in the `pros` data frame called *bot* and *surf*. We have two new processes *O2_exch*, and *O2_cons* and the flags in the corresponding columns are set to TRUE:

Table 12: Data frame 'pros': Declaration of processes.

name	unit	description	expression	surf	bot	sedi
growth	g/m^3/d	growth of algae	$C \cdot mu\_max \cdot HPO4/(HPO4 + K\_P) \cdot par/(par + K\_par)$			
death	g/m^3/d	death of algae	$C \cdot k\_death$			
sed	g/m^3/s	sinking	v_sed			TRUE
O2_exch	g/m^3/d	exchange of Oxygen at the surface	$v\_O2 \cdot (exp(7.7117 - 1.31403 \cdot log(Temp + 45.93)) \cdot (p/101325) - O2)$	TRUE		
O2_cons	g/m^3/d	consumption of Oxygen in the pelagial	$O2/(O2 + K\_O2) \cdot k\_O2\_cons$		TRUE	

We declared the additional parameters for the oxygen exchange velocity, the constant consumption in the sediment, and the half-saturation concentration of oxygen limiting the oxygen consumption in the sediment:

Table 13: Data frame `pars`: Declaration of model parameters.

name	unit	description	default
mu_max	1/s	maximum growth rate	1.0e-05
K_P	W/m^2	half saturation of photosyntetic flux	2.0e-02
k_death	1/s	death rate	2.0e-06
a_P	gP/gDM	phosphorus content of phytoplankton	5.0e-02
K_par	W/m^2	half saturation of photosyntetic flux	2.7e+01
v_sed	m/s	sedimentation velocity	1.0e-06
v_O2	1/s	speed of oxygen transfer	1.0e-05
k_O2_cons	1/s/m^2	Oxygen consumption rate in sediment	5.0e-07
K_O2	gO/m^3	half saturation concentration of oxygen consumption	5.0e+00
a_O	gO/gDM	oxygen production per growth of algae	1.0e+00

We also declared the used functions *log*, and *exp*, as well as the external dependencies p (the barometric pressure at the surface), and $Temp$ (water temperature) which are needed to calculate the oxygen saturation

concentration:

Table 14: Data frame `funs`: Declaration of model functions and dependencies from the host model.

name	unit	description	dependency
par	W/m^2	Downwelling photosynthetic radiative flux	downwelling_photosynthetic_radiative_flux
p	Pa	Atmospheric Pressure	surface_air_pressure
Temp	celsius	Water temperature	temperature
exp	-	exponential function	NA
log	-	logarithmic function	NA

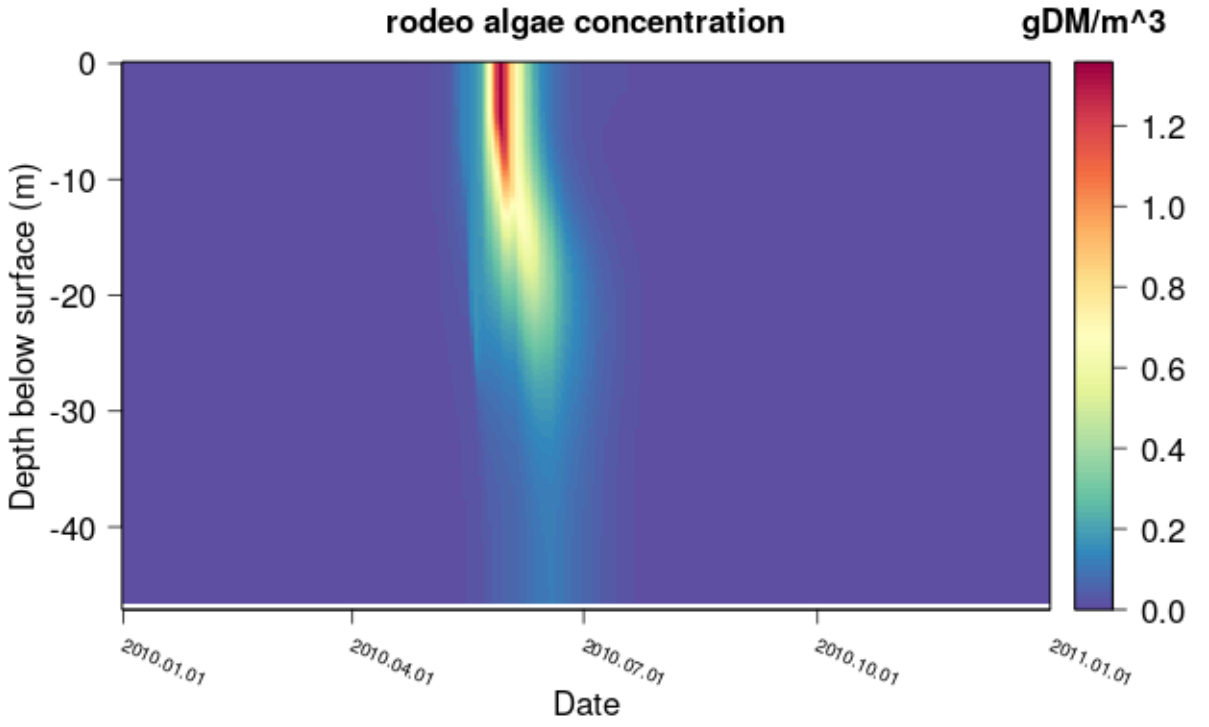
And added the new processes to the stoichiometry table:

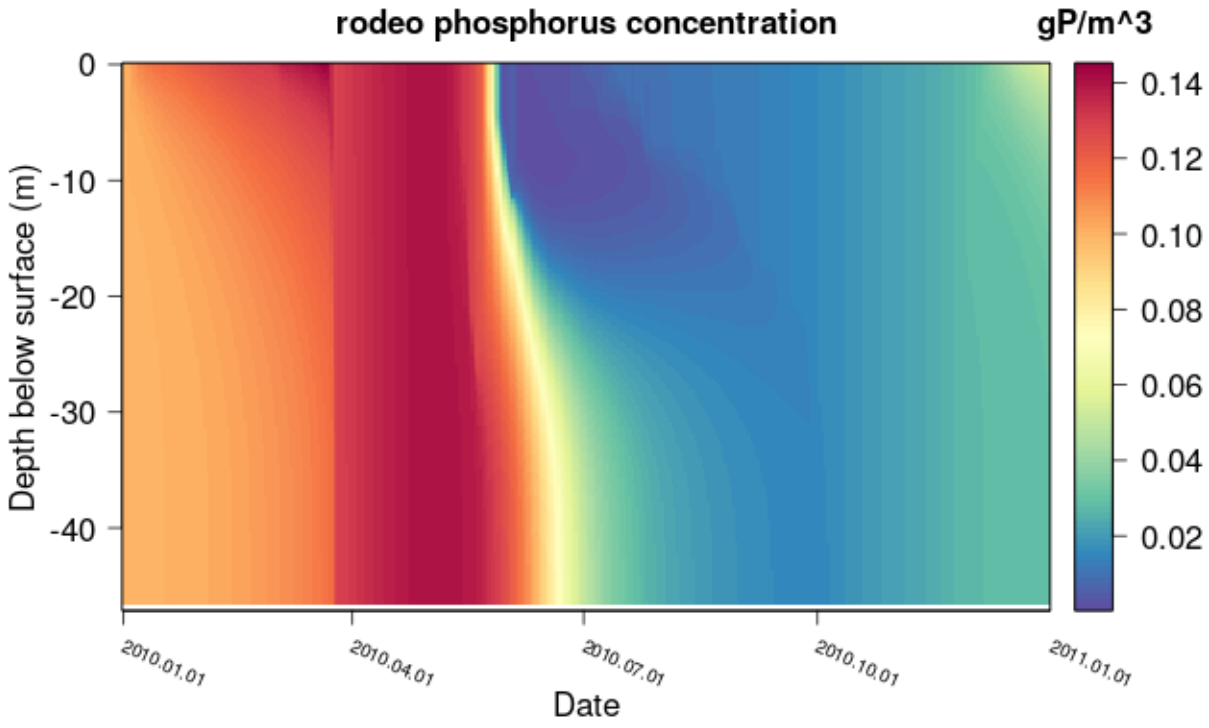
Table 15: Data frame `stoi`: Declaration of stoichiometry matrix in long format.

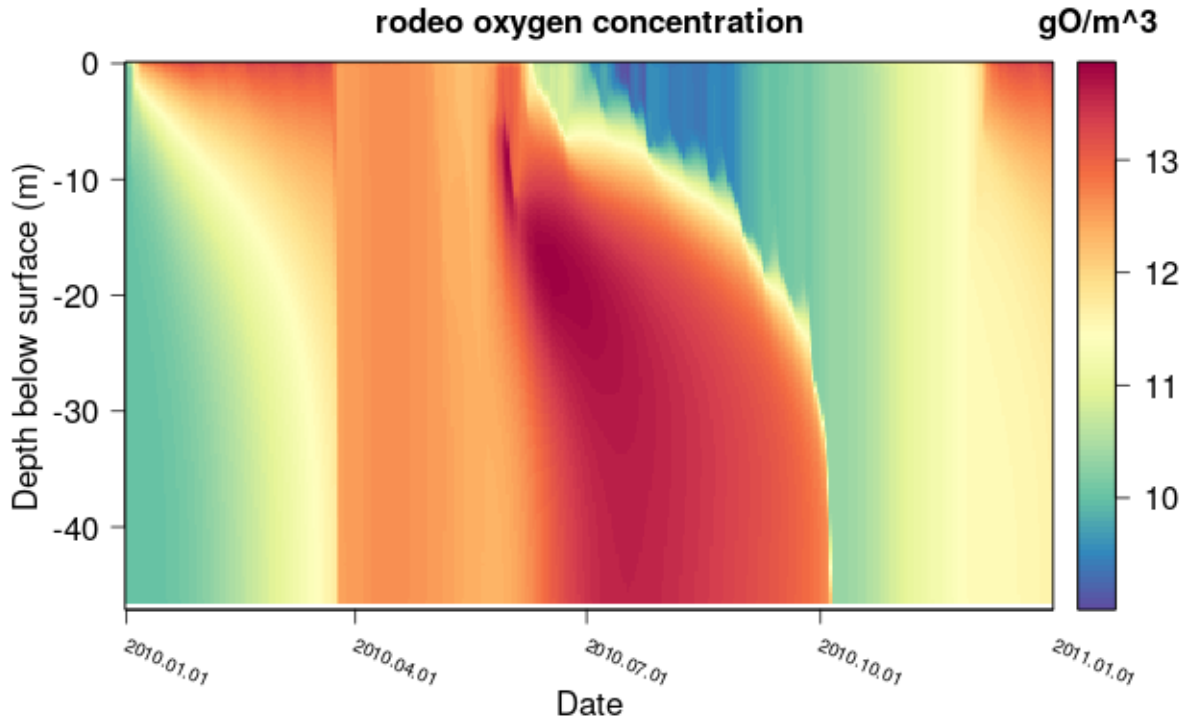
variable	process	expression
C	growth	1
C	death	-1
C	sed	-1
$HPO4$	growth	$-1 \cdot a\_P$
$O2$	O2_exch	1
$O2$	O2_cons	-1
$O2$	growth	a_O

We can generate the source code, compile *GOTM-FABM*, run the model, and plot some of the results using:

```
# create the fabm code
gen_fabm_code(vars, pars, funs, pros, stoi, "model_4.f90")

# build GOTM with the model
build_GOTM(build_dir = "build", src_dir = "gotm_src",
           fabm_file = "model_4.f90")

# run the model
system2("./gotm")

# plot the variables
plot_var("output.nc", "rodeo_C")
plot_var("output.nc", "rodeo_HPO4")
plot_var("output.nc", "rodeo_O2")
```


rodeo algae concentration
gDM/m^3
Depth below surface (m)
0
-10
-20
-30
-40
1.2
1.0
0.8
0.6
0.4
0.2
0.0
2010.01.01
2010.04.01
2010.07.01
2010.10.01
2011.01.01
Date


rodeo phosphorus concentration
gP/m^3
Depth below surface (m)
0
-10
-20
-30
-40
0.14
0.12
0.10
0.08
0.06
0.04
0.02
2010.01.01
2010.04.01
2010.07.01
2010.10.01
2011.01.01
Date



3.3.4 Sediment or surface attached state variables

As mentioned before *FABM* recognizes three spatial domains: open water, surface, and sediment. Like Processes, state variables can also be attached to one of these domaines (e.g. sedimented particulated organic matter). To demonstrate this feature we will include two more state variables in our model; particulated organic matter (POM) and sedimented particulated organic matter ($SPOM$). Again we need to copy the spread sheet from the package:

```
ods <- system.file("extdata/examples/simple_alg_O2_POM.ods",
                   package = "rodeoFABM")
file.copy(from = ods, to = ".", recursive = TRUE)

# read in first simple model
vars <- read_ods("simple_alg_O2_POM.ods", sheet = "vars")
pars <- read_ods("simple_alg_O2_POM.ods", sheet = "pars")
funs <- read_ods("simple_alg_O2_POM.ods", sheet = "funs")
pros <- read_ods("simple_alg_O2_POM.ods", sheet = "pros")
stoi <- read_ods("simple_alg_O2_POM.ods", sheet = "stoi")
```

We added the two new state variables POM and $SPOM$ and declared $SPOM$ as bottom bound state variable by adding another column to the `vars` data frame called *bot* and set it to $TRUE$ for all bottom bound state variables and to NA (empty) or $FALSE$ for all others. Surface bound state variables can be declared in the same manner using a column named *surf*.

Table 16: Data frame `vars`: Declaration of state variables.

name	unit	description	default	bot
C	gDM/m^3	algae concentration	0.0	NA
$HPO4$	gP/m^3	phosphorus concentration	0.1	NA
$O2$	gO/m^3	oxygen concentration	10.0	NA

name	unit	description	default	bot
POM	gDM/mˆ3	particulated organic matter	0.0	NA
$SPOM$	gDM/mˆ2	sedimented particulated organic matter	0.0	TRUE

Looking at the stoichiometry table we can see that the death of algae generates POM, which settles down, and sediments to the ground to become $SPOM$. Both POM and $SPOM$ are mineralized, releasing $HPO4$ but the mineralization is faster in the sediment (see *pars* table). We added the new sinking, sedimentation, and mineralization processes to the `pros` data frame:

Table 17: Data frame 'pros': Declaration of processes.

name	unit	description	expression	surf	bot	sedi
growth	gDW/mˆ3/d	growth of algae	$C \cdot mu\_max \cdot (HPO4)/(HPO4 + K\_P) \cdot (par)/(par + K\_par)$			
death	gDW/mˆ3/d	death of algae	$C \cdot k\_death$			
sed_ALG	gDW/mˆ3/s	sinking of algae	v_sed_ALG			TRUE
O2_exch	gO/mˆ3/d	exchange of Oxygen at the surface	$v\_O2 \cdot (exp(7.7117 - 1.31403 \cdot log(Temp + 45.93)) \cdot (p)/(101325) - O2)$	TRUE		
O2_cons	gO/mˆ3/d	consumption of Oxygen in the pelagial	$(O2)/(O2 + K\_O2) \cdot k\_O2\_cons$		TRUE	
sed_POM	gDW/mˆ3/s	sinking of POM	v_sed_POM			TRUE
miner_POM	gDW/mˆ3/s	mineralization of POM	$POM \cdot k\_miner\_POM \cdot (O2)/(O2 + K\_miner\_O2)$			
miner_SPOM	gDW/mˆ3/s	mineralization of SPOM	$SPOM \cdot k\_miner\_SPOM \cdot (O2)/(O2 + K\_miner\_O2)$		TRUE	
set_POM	gDW/mˆ3/s	settling of POM	$v\_sed\_POM \cdot POM$		TRUE	

And we adapted the stoichiometry table:

Table 18: Data frame `stoi`: Declaration of stoichiometry matrix in long format.

variable	process	expression
C	growth	1
C	death	-1
C	sed_ALG	-1
$HPO4$	growth	$-1 \cdot a\_P$
$HPO4$	miner_POM	a_P
$HPO4$	miner_SPOM	a_P
$O2$	O2_exch	1
$O2$	O2_cons	-1
$O2$	growth	a_O
$O2$	miner_POM	$-1 \cdot a\_miner$
$O2$	miner_SPOM	$-1 \cdot a\_miner$
POM	sed_POM	-1
POM	set_POM	-1
POM	death	1
POM	miner_POM	-1
$SPOM$	set_POM	1
$SPOM$	miner_SPOM	-1

We declared the new parameters for the sinking velocity, the mineralization kinetic, and the half-saturation concentration limiting the mineralization:

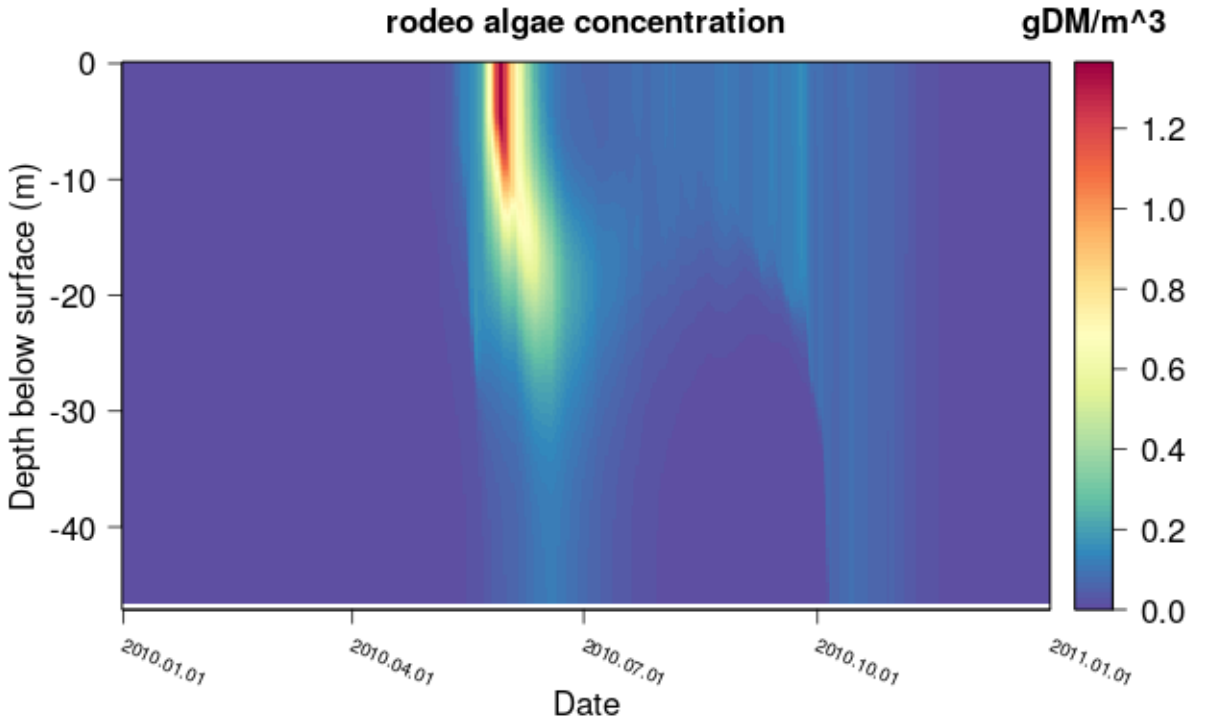
Table 19: Data frame `pars`: Declaration of model parameters.

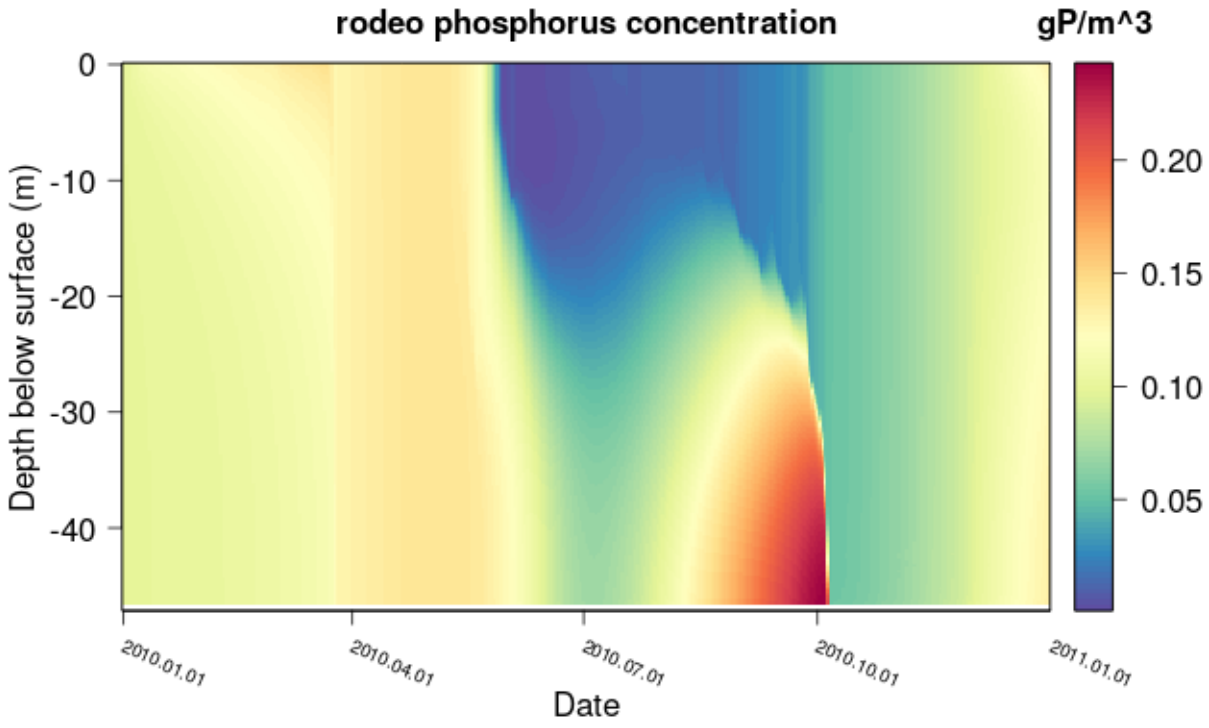
name	unit	description	default
mu_max	1/s	maximum growth rate	1.0e-05
K_P	W/mˆ2	half saturation of photosyntetic flux	2.0e-02
k_death	1/s	death rate	2.0e-06
a_P	gP/gDM	phosphorus content of phytoplankton	5.0e-02

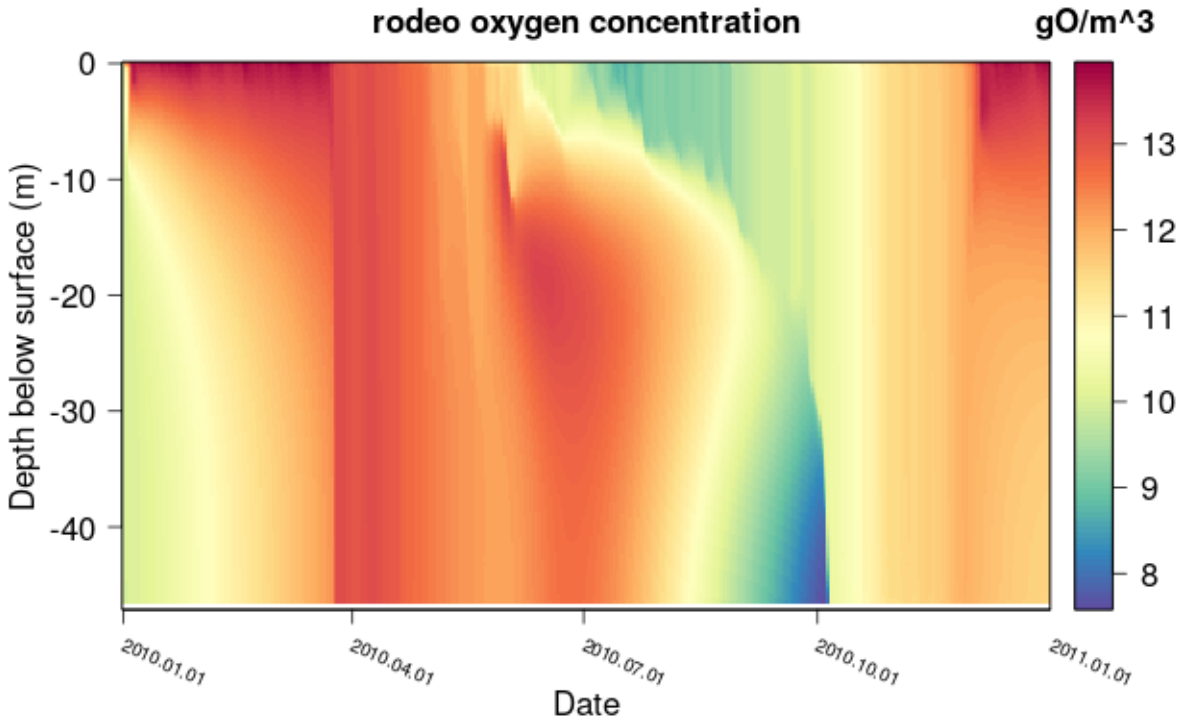
name	unit	description	default
K_par	W/mˆ2	half saturation of photosyntetic flux	2.7e+01
v_sed_ALG	m/s	sedimentation velocity of algae	1.0e-06
v_O2	1/s	speed of oxygen transfer	1.0e-04
k_O2_cons	1/s/mˆ2	Oxygen consumption rate in sediment	5.0e-07
K_O2	gO/mˆ3	half saturation concentration of oxygen consumption	5.0e+00
a_O	gO/gDM	oxygen production per growth of algae	1.0e+00
v_sed_POM	m/s	sedimentation velocity of POM	2.0e-06
K_miner_O2	gO/mˆ3	half saturation concentration of oxygen for mineralization	3.0e+00
k_miner_POM	1/s	maximum mineralization rate of POM	0.0e+00
k_miner_SPOM	1/s	maximum mineralization rate of SPOM	3.0e-07
a_miner	gO/gDM	oxygen consumption per oxygenation of POM/SPOM	1.0e+00

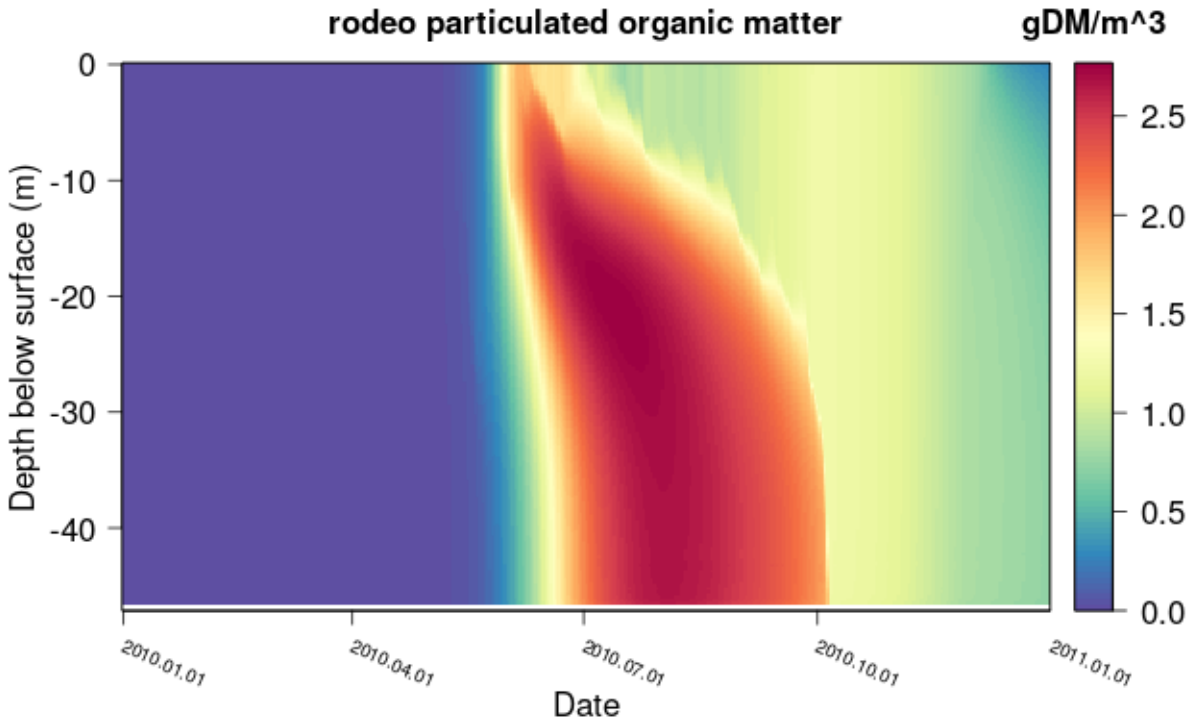
We can create fortran source code, compile *GOTM-FABM*, run the model, and plot the results using:

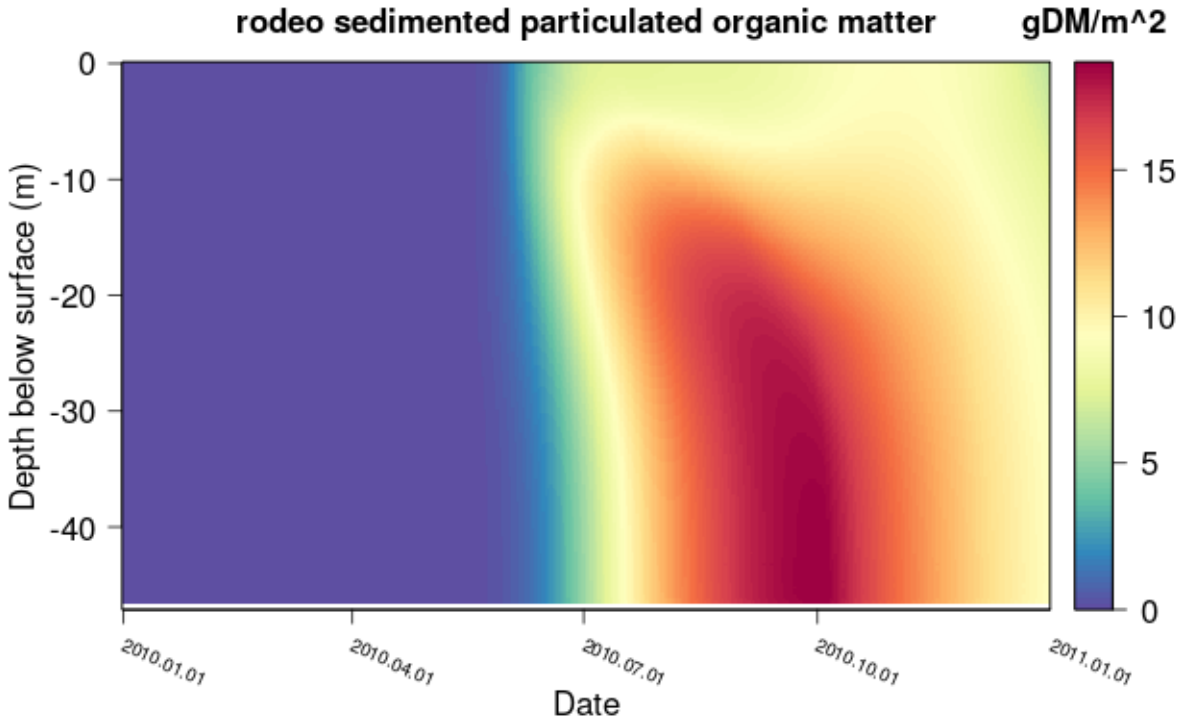
```
# create the fabm code
gen_fabm_code(vars, pars, funs, pros, stoi, "model_5.f90")

# build GOTM with the model
build_GOTM(build_dir = "build", src_dir = "gotm_src",
           fabm_file = "model_5.f90")

# run the model
system2("./gotm")

# plot the variables
plot_var("output.nc", "rodeo_C")
plot_var("output.nc", "rodeo_HPO4")
plot_var("output.nc", "rodeo_O2")
plot_var("output.nc", "rodeo_POM")
plot_var("output.nc", "rodeo_SPOM")
```


rodeo algae concentration
gDM/m^3
Depth below surface (m)
0
-10
-20
-30
-40
1.2
1.0
0.8
0.6
0.4
0.2
0.0
2010.01.01
2010.04.01
2010.07.01
2010.10.01
2011.01.01
Date


rodeo phosphorus concentration
gP/m^3
Depth below surface (m)
0
-10
-20
-30
-40
0.20
0.15
0.10
0.05
2010.01.01
2010.04.01
2010.07.01
2010.10.01
2011.01.01
Date


rodeo oxygen concentration
gO/m^3
Depth below surface (m)
0
-10
-20
-30
-40
13
12
11
10
9
8
2010.01.01
2010.04.01
2010.07.01
2010.10.01
2011.01.01
Date


rodeo particulated organic matter
gDM/m^3
Depth below surface (m)
0
-10
-20
-30
-40
2.5
2.0
1.5
1.0
0.5
0.0
2010.01.01
2010.04.01
2010.07.01
2010.10.01
2011.01.01
Date



4 Additional features

4.1 State variable arguments

There are a few additional arguments for state variables that can be defined in *FABM*. In order to use them a new column in the state variable data frame needs to be added with exactly the name.

- *minimum*: minnimum allowed value for the state variable (used in the numerical solver)
- *maximum*: maximum allowed value for the state variable (used in the numerical solver)
- *specific_light_extinction*: specific light extinction coefficient of this variable
- *no_precipitation_dilution*: the variable is not diluted by precipitation (logical)
- *no_river_dilution*: the variable is not diluted by river inflows (logical)

4.2 Initial values for the state variables

By default the initial values for the *FABM* sate variables are constant throughout the whole profile. With some tinkering we can set any profide we want as the initial values. Therefore, we need to have (a) text file(s) with (the) profiles that you want to initialise and install the R packages `ncdf4`, `data.table`, `gotmtools` from the AEMON-J github. The approach is to first run *GOTM* with 0 time steps (stop date = start date). After a run with GOTM, a `restart.nc` file is created, that can be use to restart a simulation with the same settings that ended the previous simulation. By running with 0 time steps, this file contains the "standard" initial values, including the ones in out biogeochemical model. Then we need to replaces the homogeneous initial profiles in the `restart.nc` file by our specified profiles using the `ncdf4` librarie. Lastly, we need to set the `restart` option in the `gotm.yaml` file to "true". If we run gotm now, it will run with the initial profiles for our biogeochemical model (note that we'll have to rerun this approach every time before we want to run GOTM, because every new GOTM run overwrites the `restart.nc` file). Alternatively we can save the created `restart.nc` file e.g. as `restart_init_profiles.nc` and use this file to override the `restart.nc` before we run GOTM.

4.3 Defining own functions

4.3.1 Defining functions in the *funs* data frame

It is possible to define our own functions and call them. If the function is simple i.e. can be calculated in one line of code (e.g. limiting functions for algae growth) it can be defined from the *expressions* column of the *pros* data frame. In order to define own functions two additional columns are needed in the *funs* data frame: `expression` and `arguments`. Similar to the *pros* data frame the `expression` column gives the mathematical expression to calculate. The `arguments` column gives all input arguments that the functions uses, in the same order they are supplied during function calls (e.g. in the *expression* column of the *pros* data frame), separated by commas (",").

Using this we could e.g. implement the monod function $f_{monod} = \frac{C}{C+K}$ by changing the *funs* data frame to:

Table 20: Data frame 'funs': Declaration of model functions and dependencies from the host model.

name	unit	description	dependency	expression	arguments
par	W/m^2	Downwelling photosynthetic radiative flux	*downwelling_photosynthetic_radiative_flux*		
p	Pa	Atmospheric Pressure	*surface_air_pressure*		
Temp	celsius	Water temperature	*temperature*		
exp	-	exponential function			
log	-	logarithmic function			
f_monod	-	Monod funciton		C/(C + K)	C, K

Now we can use the function in the `expression` column of the *pros* data frame e.g. by replacing:

`C · mu_max · HP O4/(HP O4 + K_P ) · par/(par + K_par)` with

`C · mu_max · f_monod(HPO4, K_P · f_monod(par, K_par)`

in the `expression` column of the growth of algae.

4.3.2 Defining functions in external fortran files

More complex functions can be supplied as external fortran code. Two additional columns are needed in the *funs* data frame: `file` and `module`. They give the name of the source code file and the name of the module, which is then loaded in the main source code. This feature is still experimental and might lead to errors!

4.4 Automatic model documentation

If wanted `rodeoFABM` can automatically generate LaTeX documentation of the state variables, parameter, processes and stoichometry. To do so the function `document_model()` can be used. Lets create a documentation of the final phytoplankton nutrients model from our example. In order to work we need an additional column named *tex* (you can also use another name for this column and supply the name to `document_model()` using the `tex` argument) in the data frames *vars*, *pars*, *funs*, and *pros* giving the corresponding LaTeX symbols to be used. The documentation function automatically generates LaTeX fraction, but in order for this to work all used fractions in the *expression* column of the *pros* data frame need to be in a specified format. The numerator and denominator need to be in brakets, even if they are just one single variable, number, or parameter: e.g. `(O2)/(O2 + K_O2)`. In the example spread sheet file they are allready added:

```
# see column "tex"
head(vars)
```

```
##   name    unit                          description default  bot   tex
## 1    C gDM/m^3                  algae concentration     0.0   NA     C
## 2 HPO4  gP/m^3              phosphorus concentration     0.1   NA HPO_4
## 3   O2  gO/m^3                  oxygen concentration    10.0   NA   O_2
## 4  POM gDM/m^3           particulated organic matter     0.0   NA   POM
## 5 SPOM gDM/m^2 sedimented particulated organic matter     0.0 TRUE  SPOM
```

```
# create LaTeX documentation for our model
document_model(vars, pars, pros, funs, stoi, landscape = FALSE)
```

```
##
##  finished
```

```
## [1] TRUE
```

We can see that now there are seven additional file in our worling directory:

```
grep(".*\\.tex", list.files(), value = TRUE)
```

```
## [1] "document_model.tex" "mat_stoi.tex"       "preamble-latex.tex"
## [4] "pros_expr.tex"      "tab_funs.tex"       "tab_pars.tex"
## [7] "tab_pros.tex"       "tab_stoi.tex"       "tab_vars.tex"
```

They are LaTeX tables of the models state variables (*tab_vars.tex*), used model parameters (*tab_pars.tex*), used functions (*tab_funs.tex*), declaration of the models processes (*tab_pros.tex*), description of the process equations (*pros_expr.tex*), the stoichiometry table (*tab_stoi.tex*), and a simple latex document that can be used to compile all of the before (*document_model.tex*).

The created expressions of the processes now look like this:

```
head(readLines("pros_expr.tex"))
```

```
## [1] "\\begin{align}"
## [2] " \\rho_{growth} =&~ C \\cdot \\mu_{max} \\cdot \\frac{HPO_4 }{ HPO_4 + K_P} \\cdot \\frac{par }{ par + K_{par}}\\\\"
## [3] " \\rho_{death} =&~ C \\cdot k_{death}\\\\"
## [4] " \\rho_{Sed,ALG} =&~ v_{sed,ALG}\\\\"
## [5] " \\rho_{O2,exch} =&~ v_{exch,O2} \\cdot \\left( \\exp \\left( 7.7117 - 1.31403 \\cdot \\log \\left( \\vartheta_z + 45.93 \\right) \\right) \\cdot \\frac{p }{ 101325} - O_2 \\right)\\\\"
## [6] " \\rho_{O2,cons} =&~ \\frac{O_2 }{ O_2 + K_{O2}} \\cdot k_{O2,cons}\\\\"
```

and compiled they look like this:

$$\rho_{growth} = C \cdot \mu_{max} \cdot \frac{HPO_4}{HPO_4 + K_P} \cdot \frac{par}{par + K_{par}} \tag{1}$$

$$\rho_{death} = C \cdot k_{death} \tag{2}$$

$$\rho_{Sed,ALG} = v_{sed,ALG} \tag{3}$$

$$\rho_{O2,exch} = v_{exch,O2} \cdot \left(\exp\left(7.7117 - 1.31403 \cdot \log\left(\vartheta_z + 45.93\right)\right) \cdot \frac{p}{101325} - O_2 \right) \tag{4}$$

$$\rho_{O2,cons} = \frac{O_2}{O_2 + K_{O2}} \cdot k_{O2,cons} \tag{5}$$

$$\rho_{Sed,POM} = v_{sed,POM} \tag{6}$$

$$\rho_{Miner,POM} = POM \cdot k_{miner,POM} \cdot \frac{O_2}{O_2 + K_{miner,O2}} \tag{7}$$

$$\rho_{Miner,SPOM} = SPOM \cdot k_{miner,SPOM} \cdot \frac{O_2}{O_2 + K_{miner,O2}} \tag{8}$$

$$\rho_{Set,POM} = v_{sed,POM} \cdot POM \tag{9}$$

References

Bruggeman, Jorn, and Karsten Bolding. 2014. "A General Framework for Aquatic Biogeochemical Models." *Environmental Modelling & Software* 61 (November): 249–65. https://doi.org/10.1016/j.envsoft.2014.04.002.

Burchard, Hans, Karsten Bolding, Wilfried Kühn, Andreas Meister, Thomas Neumann, and Lars Umlauf. 2006. "Description of a Flexible and Extendable Physical–Biogeochemical Model System for the Water Column." *Journal of Marine Systems* 61 (3): 180–211. https://doi.org/https://doi.org/10.1016/j.jmarsys.2005.04.011.

Kneis, David, Thomas Petzoldt, and Thomas U. Berendonk. 2017. "An R-Package to Boost Fitness and Life Expectancy of Environmental Models." *Environmental Modelling & Software* 96 (October): 123–27. https://doi.org/10.1016/j.envsoft.2017.06.036.