R package LakeEnsemblR: Basic Use and Sample Applications

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Contents

1 Included models

LakeEnsemblR currently includes the following models: GLM (Hipsey et al. (2019)), FLake (Mironov (2008)), GOTM (Umlauf, Bolding, and Burchard (2005)), Simstrat (Goudsmit et al. (2002)), and MyLake (Saloranta and Andersen (2007)).

2 Introduction

LakeEnsemblR is an R package that lets you run multiple one-dimensional physical lake models.

The settings for a model run are controlled by one centralised, "master" configuration file in YAML format. In this configuration file, you can set all the specifications for your model run, including start and end time, time steps, links to meteorological forcing and bathymetry files, etc. The package then converts these settings to the configuration files required by each model, through the `export_config` function. This sets up all models to run with the settings specified by the user, and the models are then run through the `run_ensemble` function. A netcdf file is created with the outputs of all the models, and the package provides functions to extract and plot this data.

Part of the design philosophy of LakeEnsemblR is that all input is given in a standardized format. This entails standard column names (which includes units), comma-separated ASCII files, and a DateTime format using the international standard format (ISO 8601), which is `YYYY-mm-dd HH:MM:SS`, for example `2020-04-03 09:00:00`. In this document, we will explain what the required files are and in what format they need to be. We also advise you to look at the provided example files, and at the templates provided with the R package (to be found in `package/inst/extdata`, or extracted by the function `get_template`).

3 Installation

The code of LakeEnsemblR is hosted on the AEMON-J Github page (https://github.com/aemon-j/LakeEnsemblR), and can be installed using the `devtools` package

```
devtools::install_github("aemon-j/LakeEnsemblR)
```

The package relies on multiple other packages that also need to be installed. Most notably, to run the multiple models, it requires the packages FLakeR, GLM3r, GOTMr, SimstratR, and MyLakeR. These packages run the individual models, and contain ways of running the models for the platforms Windows, MacOS, or UNIX, through either executables, or by having the model code in R.

4 The LakeEnsemblR configuration file

In this section, we go through the LakeEnsemblR configuration file. This file controls the settings with which the models are run. It is written in YAML (Yaml Ain't Markup Language) format, and can be opened by text-editors such as Notepad or Notepad++. Although not needed to use LakeEnsemblR, you can read this file into R with the `configr` package (`read.config` function). Within LakeEnsemblR, we provide the `get_yaml_value` and `input_yaml` functions to get and input values into this file type.

There is an LakeEnsemblR configuration file provided in the example dataset in the package (`LakeEnsemblR::get_template("LakeEnsemblR_config")`) or you can download a copy from GitHub here.

4.1 Location

The first section is "Location". Here you specify the name, latitude and longitude, elevation, maximum depth, and initial depth.

You also need to provide a link to the hypsograph (i.e. surface area per depth) file. As in the rest of the configuration file, all links to files are relative to the `folder` argument in the LakeEnsemblR functions (default is the R working directory). We strongly advise to set the working directory to the location of the LER config file, and link to the files relative to this directory (we explain this further in the chapter "Workflow" of this vignette). For example, if your hypsograph file is called `hypsograph.csv` and in the same folder as the LER config file, the corresponding line in the LER config file would look like

```
  hypsograph: hypsograph.csv
```

The data needs to be a comma-separated file (.csv) where 0m is the surface and all depths are reported as positive, in meters. Area needs to be in meters squared. The column names *must* be `Depth_meter` and `Area_meterSquared`

Example of data:

```
Depth_meter,Area_meterSquared
0,3931000
1,3688025
2,3445050
3,3336093.492
4,3225992.455
5,3133491.11
6,3029720
...
```

4.2 Time

In the "Time" section, you fill in the start and end date of the simulation, and the model time step. `time_step` indicates the model integration time step, so each time step that the model performs a calculation.

4.3 Config files

In this section, you link to the model-specific configuration files. Templates of these can be found in in the package (`get_template("FLake_config")`, `get_template("GLM_config")`, etc. all available templates can be shown using `get_template()`) or you can download a copy from GitHub here. The setup of LakeEnsemblR is such that you will usually not have to access these files, as most settings are regulated through the LER "master" config file. However, should you want to change some of the more specialised settings in each model, that is possible.

4.4 Light

Here you can either give a value for Kw (light extinction coefficient) in 1/m, or give the link to a file, where you can vary Kw over time (template available using `get_template("Light extinction")`). The file must be a comma-separated file (.csv) with the two columns `datetime` and `Extinction_Coefficient_perMeter` containing the date in ISO 8601 format (`YYYY-mm-dd HH:MM:SS`) and corresponding Kw value in 1/m.

4.5 Observations

If you have observations of water temperature or ice cover, you can fill them in here. These will be used in plotting, and in case of water temperature potentially in initialising the temperature profile at the start of the simulation (see next section).

For water temperature, the data needs to be a comma separated values (.csv) file where the datetime column is in the format `YYYY-mm-dd HH:MM:SS`. Depths are positive and relative to the water surface. Water temperature is in degrees Celsius. The column names *must* be `datetime`, `Depth_meter` and `Water_Temperature_celsius` (templates available).

Example of data:

```
datetime,Depth_meter,Water_Temperature_celsius
2004-01-05 00:00:00,0.9,6.97
2004-01-06 00:00:00,2.5,6.71
2004-01-07 00:00:00,5,6.73
2004-01-08 00:00:00,8,6.76
...
```

For ice height, the data must also be a comma separated values (.csv) file, with datetime column in format `YYYY-mm-dd HH:MM:SS` and has the column name `datetime`. Ice height must be provided in meters and the column must be named `Ice_Height_meter`.

Example of data:

```
datetime, Ice_Height_meter
2004-01-01 00:00:00,0.3
2004-01-02 00:00:00,0.3
2004-01-03 00:00:00,0.35
...
```

4.6 Input

In the "Input" section, you give information about the initial temperature profile, meteorological forcing, and ice.

Firstly, you can give the initial temperature profile with which to start the simulation (link to .csv file, template available using `get_template("Initial temperature profile")`). If you leave it empty, the water temperature observations will be used, provided you have an observation on the starting time of your simulation.

Secondly, you give the link to the file with your meteorological data. The data needs to be a comma separated values (.csv) file where the datetime column is in the format `YYYY-mm-dd HH:MM:SS`. See Table 1 for the list of variables, units and column names. The `time_zone` setting has not been implemented yet.

Lastly, you can specify if you want to use the ice modules that are present in some of the models.

4.7 Inflows

Specify if you want to add inflows to your simulation. If yes, you need to link to a file with the inflow data. The data needs to be a comma separated values (.csv) file where the datetime column is in the format `YYYY-mm-dd HH:MM:SS`. Flow discharge, water temperature, and salinity need to be specified. The column names *must* be `datetime`, `Flow_metersCubedPerSecond`, `Water_Temperature_celsius`, and `Salinity_practicalSalinityUnits` (template available using `get_template("Inflow")`).

Example of data:

```
datetime,Flow_metersCubedPerSecond,Water_Temperature_celsius,Salinity_practicalSalinityUnits
2005-01-01 00:00:00,5.62,6.96,0.00
2005-01-02 00:00:00,2.32,6.00,0.00
2005-01-03 00:00:00,1.77,8.44,0.00
2005-01-04 00:00:00,4.64,7.27,0.00
...
```

Description	Units	Column Name	Status
Downwelling longwave radaiation	W/m2	Longwave_Radiation_Downwelling_wattPerMeterSquared	If not provided,it is calculated internally from air temperature, cloud cover and relative humidity/dewpoint temperature
Downwelling shortwave radaiation	W/m2	Shortwave_Radiation_Downwelling_wattPerMeterSquared	Required
Cloud cover	-	Cloud_Cover_decimalFraction	If not provided,it is calculated internally from air temperature, short-wave radiation, latitude, longitude, elevation and relative humidity/dewpoint temperature
Air temperature	°C	Air_Temperature_celsius	Required
Relative humidity	%	Relative_Humidity_percent	If not provided,it is calculated internally from air temperature and dewpoint temperature
Dewpoint temperature	°C	Dewpoint_Temperature_celsius	If not provided,it is calculated internally from air temperature and relative humidity
Wind speed at 10m	m/s	Ten_Meter_Elevation_Wind_Speed_meterPerSecond	Either wind speed or u and v vectors is required
Wind direction at 10m	°C	Ten_Meter_Elevation_Wind_Direction_degree	Not required, but if provided u and v vectors are calculated internally
Wind u-vector at 10m	m/s	Ten_Meter_Uwind_vector_meterPerSecond	Either wind speed or u and v vectors is required
Wind v-vector at 10m	m/s	Ten_Meter_Vwind_vector_meterPerSecond	Either wind speed or u and v vectors is required
Precipitation	m/s	Precipitation_meterPerSecond	Not strictly required but is important for mass budgets in some models
Rainfall	m/s	Rainfall_meterPerSecond	Required
Snowfall	m/day	Snowfall_meterPerDay	If not provided,it is calculated internally from rain when air temperature < 0 degC
Sea level pressure	Pa	Sea_Level_Barometric_Pressure_pascal	Not required
Surface level pressure	Pa	Surface_Level_Barometric_Pressure_pascal	Required
Vapour pressure	mbar	Vapor_Pressure_milliBar	If not provided,it is calculated internally from air temperature and relative humidity/dewpoint temperature

Table 1: Description of meteorological variables used within LakeEnsemblR with units and required column names.

4.8 Output

In the "Output" section, you specify how the output should look like. Currently, only the netcdf option is in place. You can specify the depth interval of the output, and the frequency. Also specify what variables should be in the output (currently only "temp" and "ice_height").

4.9 Biogeochemistry

Currently not implemented

4.10 Model parameters

All models in LakeEnsemblR have different parameterizations. In this section, you can set the value of any parameter in one of the model-specific configuration files.

You can give either only the name of the parameter, but if needed you can also provide the name of the section in which the parameter occurs, separated by a `/`. For example for GOTM's k_min parameter:

```
GOTM:
  k_min: 3.6E-6
```

or:

```
GOTM:
  turb_param/k_min: 3.6E-6
```

4.11 Calibration

This section is used when calibrating the models. In the package, the run_LHC (Latin-Hypercube) and run_MCMC (Monte-Carlo Markov Chain) functions do this, but this is currently still in a beta-phase and this will be more clearly explained in a later version of this vignette.

5 Workflow

In this chapter, we quickly show you how your workflow with LakeEnsemblR could look like.

5.1 Setting up a directory

First, you make an empty directory for the simulations of a specific lake. In this directory, you place the LakeEnsemblR configuration file, and the necessary LakeEnsemblR-format input files (e.g. meteorology, inflow, water temperature observations, hypsograph). Within this directory, you create empty folders for each model (FLake, GLM, GOTM, Simstrat, MyLake), and in here you place the model-specific configuration files, corresponding the information you put in the `config_files` section in the LER config file.

5.2 Export_config

Then, you run the `export_config` function, which exports the settings in the LER configuration file to the model-specific configuration files. It is possible to run parts of this function, such as `export_meteo`, if the meteorological forcing is the only thing you changed, but usually you will run `export_config`.

5.3 Optional: changes in model-specific directories

Optionally, you can now go into the model-specific configuration files and make further changes. This should not be needed for regular simulations, especially since you can control parameters in the `model_parameters` section of the LER config file, but the option is there. For example, if you want to change the depth of the inflow in the Simstrat model, you could go to the Simstrat folders and make these changes manually (or through a script you wrote). It speaks for itself that these changes should be done only if you are sure this is what you need, and LakeEnsemblR does not provide further support for this.

5.4 Run_ensemble

The next step would be to call `run_ensemble`, which runs all the models. A new folder called "output" is created, in which a netcdf-file will be put with all the results from the model runs. If you are interested, each model sub-folder will also have an "output" folder, with the model-specific model output.

5.5 Example model run

See below for an example run, and some post-processing of the data.

```
# Install packages - Ensure all packages are up to date - parallel development ongoing
#install.packages("devtools")
devtools::install_github("GLEON/GLM3r")
devtools::install_github('USGS-R/glmtools', ref = 'ggplot_overhaul')
devtools::install_github("aemon-j/FLakeR", ref = "inflow")
devtools::install_github("aemon-j/GOTMr")
devtools::install_github("aemon-j/gotmtools")
devtools::install_github("aemon-j/SimstratR")
devtools::install_github("aemon-j/LakeEnsemblR")
devtools::install_github("aemon-j/MyLakeR")

# Load libraries
library(gotmtools)
library(LakeEnsemblR)

# Set working directory with example data from Lough Feeagh, Ireland
template_folder <- system.file("extdata/feeagh", package= "LakeEnsemblR")
dir.create("example") # Create example folder
file.copy(from = template_folder, to = "example", recursive = TRUE)
setwd("example/feeagh") # Change working directory to example folder

# Set models & config file
model <- c("GLM",  "FLake", "GOTM", "Simstrat", "MyLake")
config_file <- "Feeagh_master_config.yaml"

# 1. Example - creates directories with all model setup
export_config(config_file = config_file, model = model, folder = ".")

# 2. Create meteo driver files
export_meteo(config_file = config_file, model = model)

# 3. Create initial conditions
start_date <- get_yaml_value(file = config_file, label =  "time", key = "start")

export_init_cond(config_file = config_file,
                 model = model,
                 date = start_date,
                 print = TRUE)

# 4. Run ensemble lake models
wtemp_list <- run_ensemble(config_file = config_file,
                           model = c("FLake", "GLM", "GOTM", "Simstrat", "MyLake"),
                           return_list = TRUE)
```

Plotting the model outputs is very easy using the `plot_heatmap()` function:

```
g1 <- plot_heatmap("output/ensemble_output.nc")

ggsave("output/model_ensemble_watertemp.png", g1,  dpi = 300,width = 384,height = 300,
       units = "mm")
```

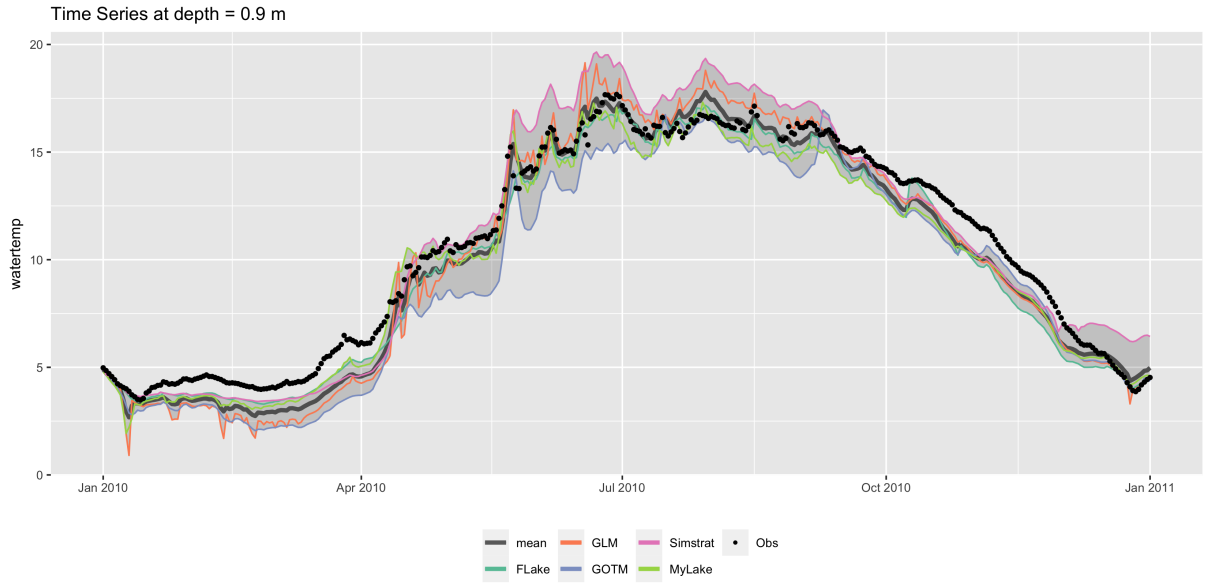
5.6 Post-processing

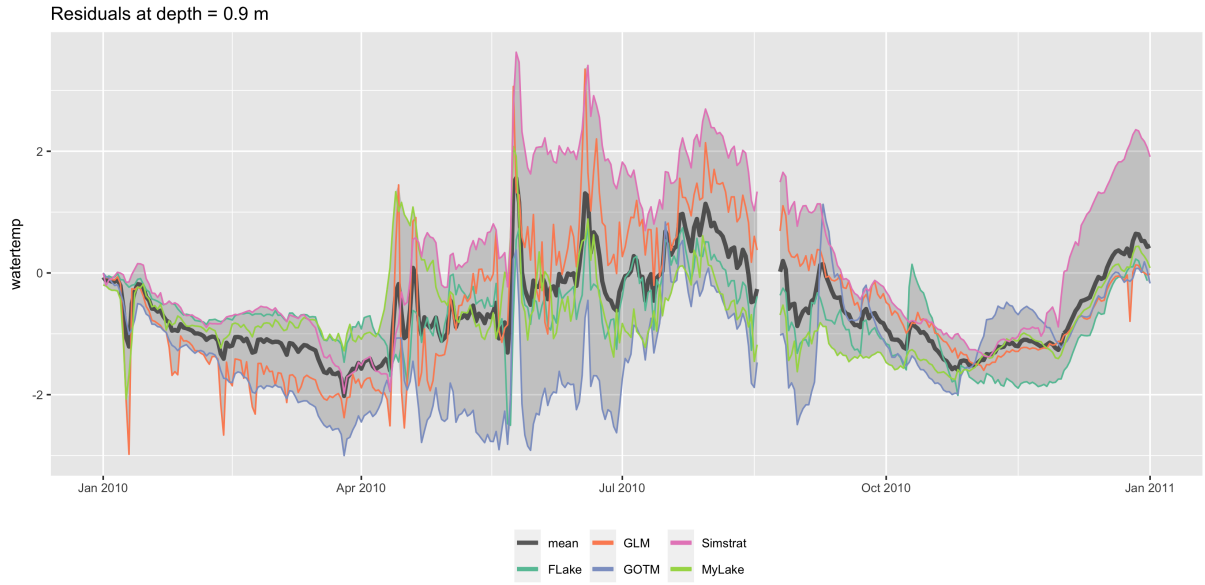
Once LakeEnsemblR did successfully run all lake models, you can either extract the output data from the netcdf file for custom analysis and plotting, or use post-processing scripts for an initial look at the output.

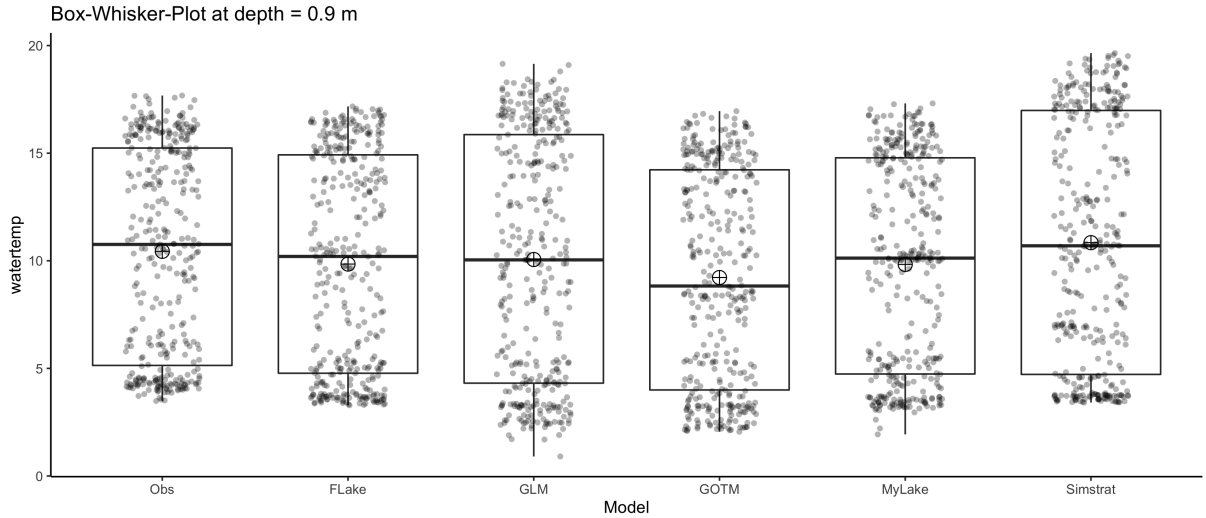
5.6.1 Quick post-processing

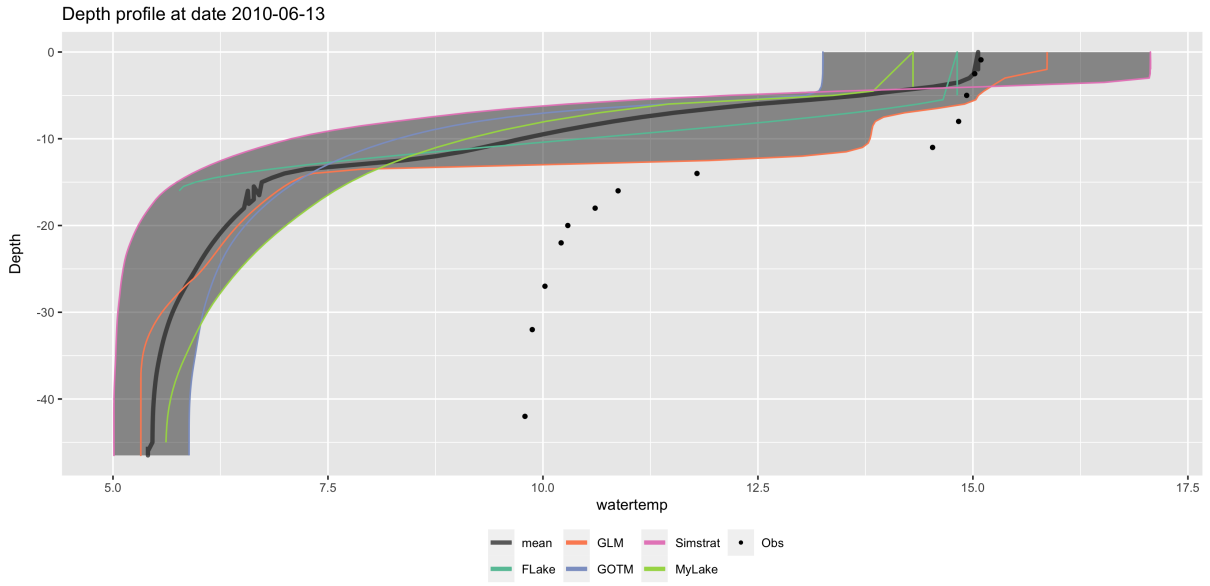
Now that the model simulations are finished, you can extract the data with `load_var`, or plot it with `plot_ensemble`. You can extract data from the netcdf file to do any further analysis. The `ncdf4` R package supports working with netcdf data in R, and the PyNcView software (https://sourceforge.net/projects/pyncview/) can be used to look at netcdf output.

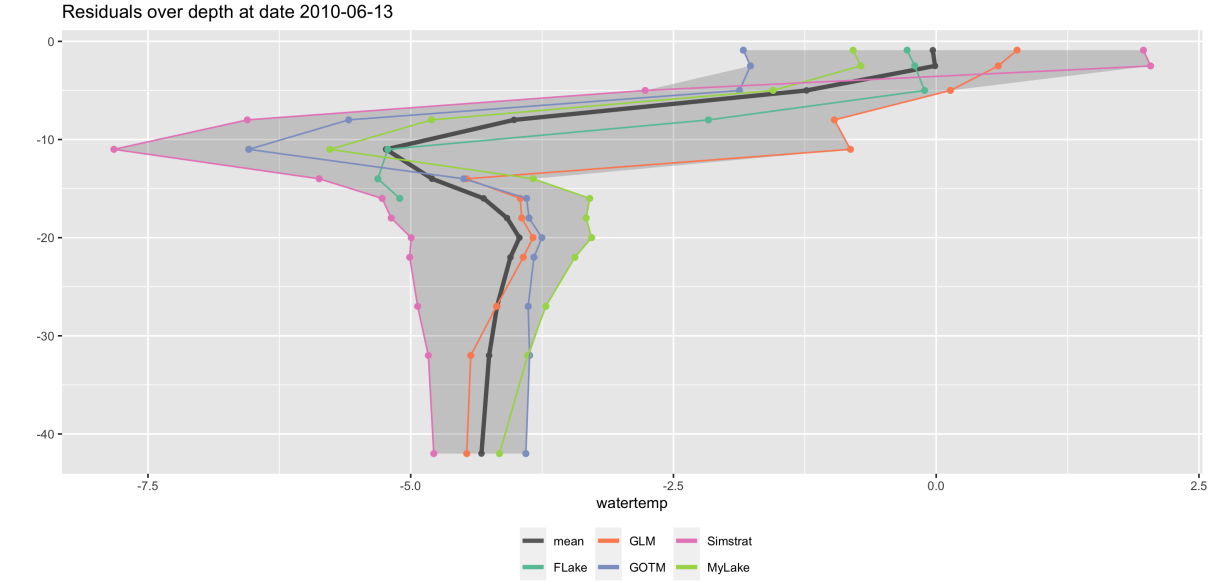
```
# Import the LEr output into your workspace
ens_out <- "output/ensemble_output.nc"

# Plot depth and time-specific results
p <- plot_ensemble(ncdf = ens_out, model = c('FLake', 'GLM',  'GOTM', 'Simstrat', 'MyLake'),
                   depth = 0.9, var = 'watertemp', date = as.POSIXct("2010-06-13", tz = "UTC"),
                   boxwhisker = TRUE, residuals = TRUE)
```

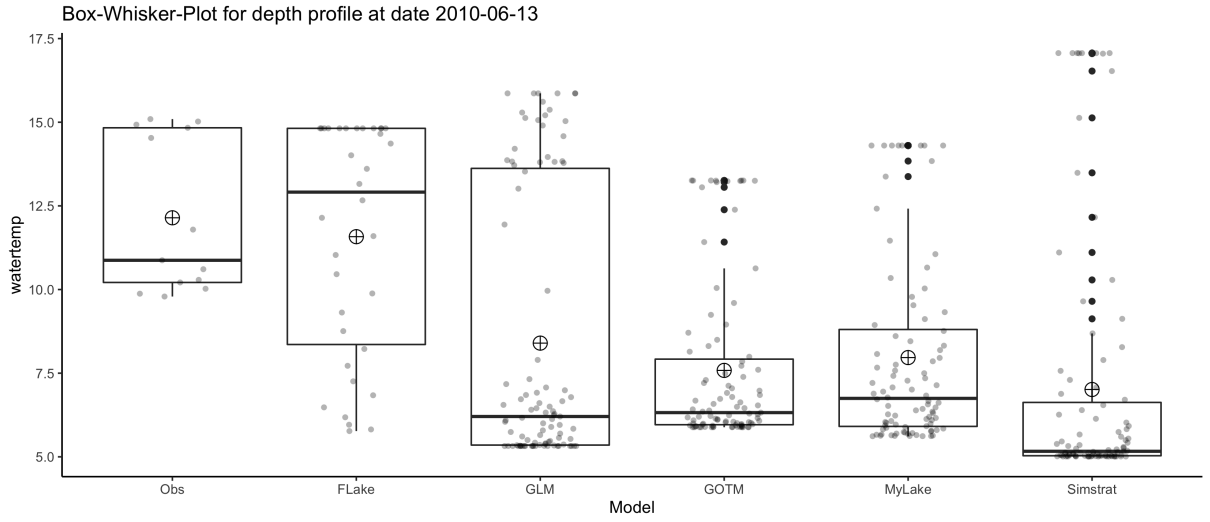

Time Series at depth = 0.9 m
watertemp
20
15
10
5
0
Jan 2010
Apr 2010
Jul 2010
Oct 2010
Jan 2011
mean
GLM
Simstrat
Obs
FLake
GOTM
MyLake


Residuals at depth = 0.9 m
watertemp
2
0
-2
Jan 2010
Apr 2010
Jul 2010
Oct 2010
Jan 2011
mean
GLM
Simstrat
FLake
GOTM
MyLake


Box-Whisker-Plot at depth = 0.9 m
watertemp
20
15
10
5
0
Obs
FLake
GLM
GOTM
MyLake
Simstrat
Model

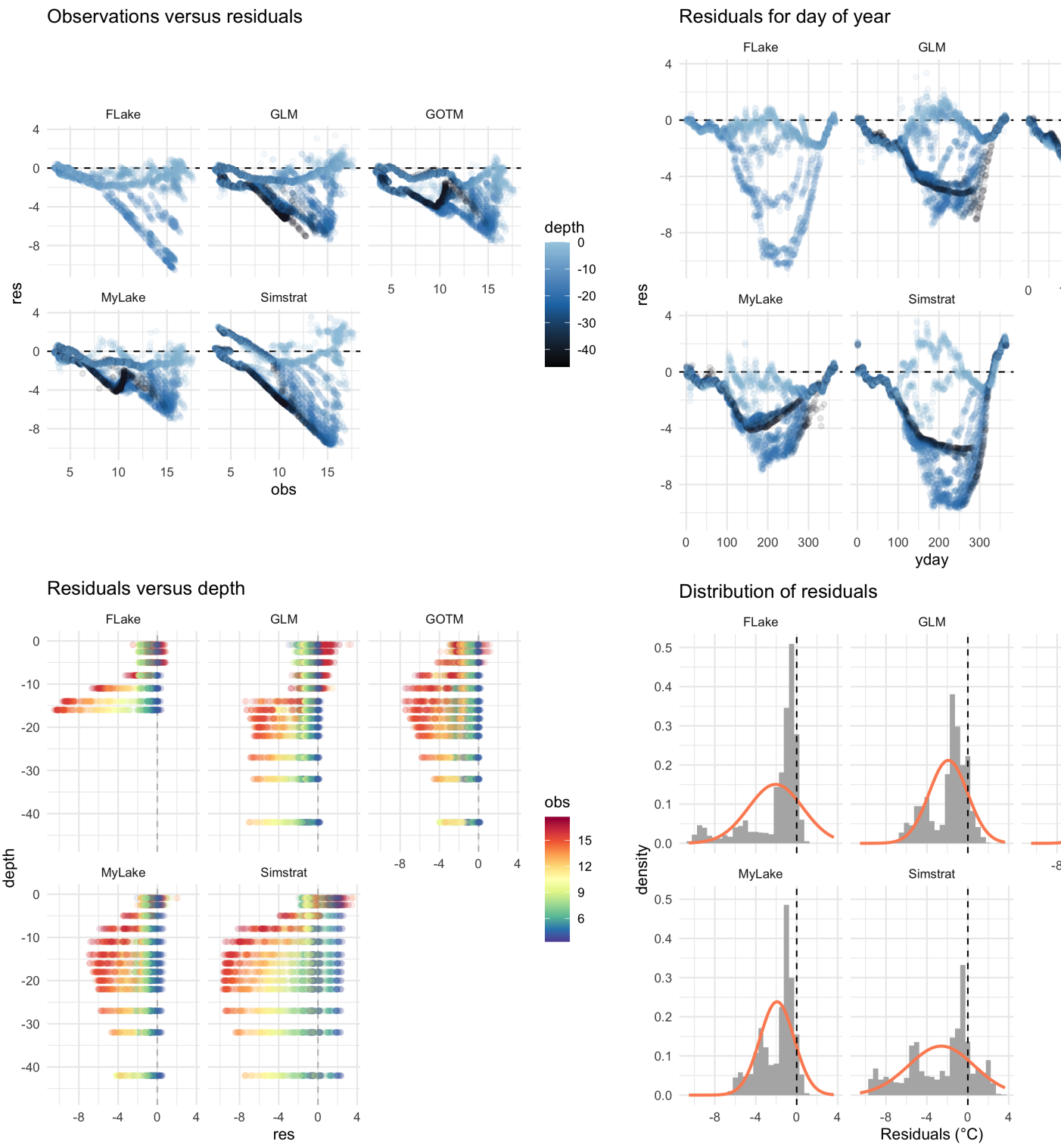

Depth profile at date 2010-06-13
Depth
watertemp
mean
GLM
Simstrat
Obs
FLake
GOTM
MyLake


Residuals over depth at date 2010-06-13
watertemp
mean
GLM
Simstrat
FLake
GOTM
MyLake


Box-Whisker-Plot for depth profile at date 2010-06-13
watertemp
Obs
FLake
GLM
GOTM
MyLake
Simstrat
Model

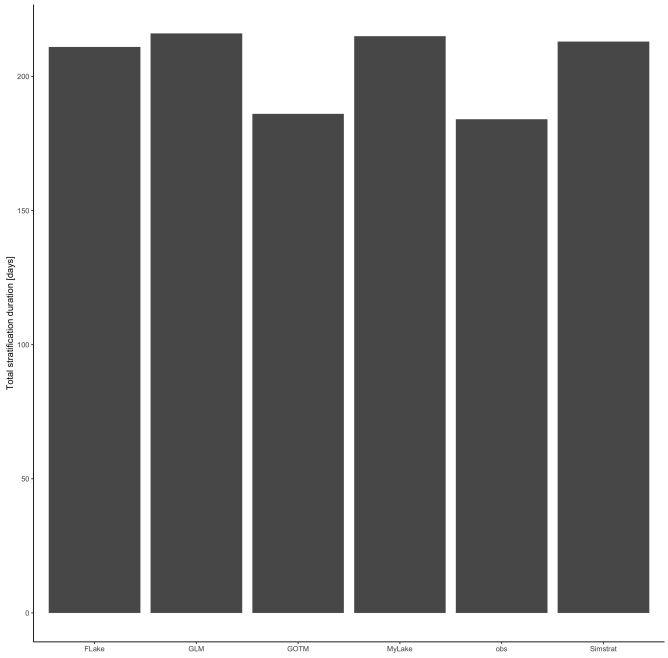
```
# Take a look at the model fits to the observed data
calc_fit(ncdf = "output/ensemble_output.nc",
         model = c("FLake", "GLM",  "GOTM", "Simstrat", "MyLake"),
         var = "watertemp")

print(calc_fit)
$FLake
      rmse      nse         r         re      nmae
1 3.356338 0.651542 0.6452533 -0.1836044 0.1877008

$GLM
      rmse       nse         r         re      nmae
1 2.677758 0.5880857 0.8791993 -0.2142704 0.2230113

$GOTM
      rmse       nse         r         re      nmae
1 2.855198 0.5303783 0.8983338 -0.2464723 0.2478081

$Simstrat
      rmse        nse        r         re      nmae
1 4.111067 0.02639042 0.653375 -0.2212801 0.2915025

$MyLake
      rmse       nse         r         re      nmae
1 2.548408 0.6258777 0.9059941 -0.1880694 0.1946865
```

```
# Take a look at the model performance against residuals, time and depth
plist <- plot_resid(ncdf = ens_out,var = "watertemp",
                    model = c('FLake', 'GLM',  'GOTM', 'Simstrat', 'MyLake'))
```



5.6.2 Further custom post-processing

```
# Load post-processed output data into your workspace
analyse_df <- analyse_ncdf(ncdf = ens_out, model = model, spin_up = NULL, drho = 0.1)

# Example plot the summer stratification period
strat_df <- analyse_df$strat

p <- ggplot(strat_df, aes(model, TotStratDur)) +
  geom_col() +
  ylab("Total stratification duration [days]") +
  xlab("") +
  theme_classic()
ggsave("output/model_ensemble_stratification.png", p,  dpi = 300, width = 284,
       height = 284, units = "mm")
```



We are currently working on a function to add new simulations (for example with a different meteorology file) to the same netcdf and including them in the analysis.

6 Citation

See

```
citation("LakeEnsemblR")
```

on how to cite this project.

Although this information is included when running the function above, we would like to repeat that in case you use and cite LakeEnsemblR, you will also need to cite the individual models that you used in your simulations.

References

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