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LakeEnsemblR: An R package that facilitates ensemble modelling of lakes

Tadhg N. Moore [a,1,*], Jorrit P. Mesman [b,c,**], Robert Ladwig [d,***], Johannes Feldbauer [e,****], Freya Olsson [f], Rachel M. Pilla [g], Tom Shatwell [h], Jason J. Venkiteswaran [i], Austin D. Delany [d], Hilary Dugan [d], Kevin C. Rose [j], Jordan S. Read [k]

[a] *Dundalk Institute of Technology, Centre for Freshwater and Environmental Studies, Dundalk, Co. Louth, Ireland*
[b] *University of Geneva, Department F.A. Forel for Environmental and Aquatic Sciences, Geneva, Switzerland*
[c] *Uppsala University, Department of Ecology and Genetics, Uppsala, Sweden*
[d] *University of Wisconsin – Madison, Center for Limnology, Madison, WI, USA*
[e] *Technische Universität Dresden, Institute of Hydrobiology, Dresden, Germany*
[f] *UK Centre for Ecology & Hydrology, Lancaster Environment Centre, Bailrigg, Lancaster, UK*
[g] *Miami University, Department of Biology, Oxford, OH, USA*
[h] *Helmholtz Centre for Environmental Research (UFZ), Department of Lake Research, Magdeburg, Germany*
[i] *Wilfrid Laurier University, Department of Geography and Environmental Studies, Waterloo, Ontario, Canada*
[j] *Rensselaer Polytechnic Institute, Department of Biological Sciences, Troy, NY, USA*
[k] *U.S. Geological Survey, Middleton, WI, USA*

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ABSTRACT

Model ensembles have several benefits compared to single-model applications but are not frequently used within the lake modelling community. Setting up and running multiple lake models can be challenging and time consuming, despite the many similarities between the existing models (forcing data, hypsograph, etc.). Here we present an R package, LakeEnsemblR, that facilitates running ensembles of five different vertical one-dimensional hydrodynamic lake models (FLake, GLM, GOTM, Simstrat, MyLake). The package requires input in a standardised format and a single configuration file. LakeEnsemblR formats these files to the input required by each model, and provides functions to run and calibrate the models. The outputs of the different models are compiled into a single file, and several post-processing operations are supported. LakeEnsemblR's workflow standardisation can simplify model benchmarking and uncertainty quantification, and improve collaborations between scientists. We showcase the successful application of LakeEnsemblR for two different lakes.

1. Introduction

Numerical process-based lake models are powerful tools to simulate processes occurring in aquatic ecosystems. These models enable the users to investigate scientific and engineering hypotheses or scenarios, which would otherwise not be feasible (or even possible) to field-test for physical, logistical, political or financial reasons. Over recent decades, the understanding of fluid dynamics and physical transport processes in lakes has improved thanks to enhanced field monitoring and intensive laboratory studies (Csanady, 1975; Imberger, 1985; Imberger and Hamblin, 1982; Imboden, 1973; Kitaigorodskii and Miropolsky, 1970; Spigel et al., 1986; Spigel and Imberger, 1980). With better empirical relationships and physical understanding of processes, the pioneer lake models that emerged from these studies were essential to addressing emerging water quality issues like eutrophication (French and Imberger, 1984).

Today, one-dimensional (1D) lake models are frequently used to characterise lake hydrodynamics. These models assume complete and

* Corresponding author.
** Corresponding author. University of Geneva, Department F.A. Forel for Environmental and Aquatic Sciences, Geneva, Switzerland.
*** Corresponding author.
**** Corresponding author.
E-mail addresses: tadhgm@vt.edu (T.N. Moore), jorrit.mesman@unige.ch (J.P. Mesman), rladwig2@wisc.edu (R. Ladwig), johannes.feldbauer@tu-dresden.de (J. Feldbauer), folsson32@ceh.ac.uk (F. Olsson), pillarm@miamioh.edu (R.M. Pilla), tom.shatwell@ufz.de (T. Shatwell), jvenkiteswaran@wlu.ca (J.J. Venkiteswaran), addelany@wisc.edu (A.D. Delany), hdugan@wisc.edu (H. Dugan), rosek4@rpi.edu (K.C. Rose), jread@usgs.gov (J.S. Read).
[1] Present address: Virginia Tech, Department of Biological Sciences, Blacksburg, VA, United States.

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instantaneous horizontal mixing. In many systems this is a reasonable assumption, because vertical thermal gradients are typically much larger than horizontal thermal gradients. The assumption holds for lakes with a small to moderate surface area that are not affected by Coriolis acceleration or other significant horizontal transport processes (Patterson et al., 1984). To model water column thermal dynamics resulting from atmospheric exchange processes, inflow entrainment and turbulence, different theoretical approaches have been developed and applied in lake models, e.g., bulk models, energy-balance approach models, and models that use a pure turbulence approach to account for mixing (Goudsmit et al., 2002). Alternative approaches apply simpler schemes to solve advection-diffusion equations or use constants for transport processes.

Since the 1980s, there has been a rapid expansion in the publication of process-based aquatic ecosystem models. However, the aquatic ecosystem community has not fully exploited the diversity of available models by comparing the performance of models against one another, which affords both the opportunity to identify technical improvements but also improve overall model predictions (Janssen et al., 2015). Critical voices still highlight the problem that modelling teams tend to 'reinvent the wheel' (Mooij et al., 2010) instead of building on existing software. The Lake Model Intercomparison Project (LakeMIP) had several key findings regarding the current state of lake modelling: (1) the majority of lake models replicate surface temperature dynamics coherently well (Stepanenko et al., 2013), (2) individual lake models clearly outperform others for specific lake sites (Thiery et al., 2014), and (3) models that explicitly incorporate sediment heating and resolve turbulence over lake depth are better suited to represent lakes in numerical meteorological studies and to research hydrodynamic processes for deep lakes (Stepanenko et al., 2013; Thiery et al., 2014). Most authors agree that open community approaches as well as publishing the model as open-source code are the best steps for sustainable development and to ensure future technical improvements (Frassl et al., 2019; Janssen et al., 2015; Read et al., 2016). Still, a lack of common community framework for model calibration, validation, and processing has resulted in few studies that quantify model performance (benchmarking) and minimal progress in improving code and applications (Arhonditsis et al., 2014; Hipsey et al., 2020).

In the 1990s, atmospheric researchers popularised the use of ensemble modeling in operational forecasting and uncertainty predictions (Parker, 2013). Ensemble modeling involves either running the same model multiple times with different settings or running multiple models on the same study site. One of the main advantages of model ensembles is that the uncertainty in the model predictions can be estimated (Trolle et al., 2014;Wu et al., 2020). This allows the modeller to assess the likelihood of occurrence of certain model predictions. Connected to this, ensemble runs of an individual model are a means of taking into account nonuniqueness (i.e. equifinality - see Beven, 2006) in parameter sets (Gal et al., 2014; Nielsen et al., 2014). The average of individual model runs from different models can be a more robust predictor than any of the individual model runs (Kobler and Schmid, 2019; Trolle et al., 2014; and sources therein). If only the "best" model is retained, valuable information in other model fits is disregarded (Baker and Ellison, 2008). An ensemble of multiple models supports the identification of methodological and technical differences and shortcomings between the different models, and covers a wide set of different parameterisations of processes. This can improve the understanding of model performance and guide future model development (Frassl et al., 2019; Janssen et al., 2015).

Model ensembles are now widely used in meteorological forecasting (Gneiting and Raftery, 2005; Leutbecher and Palmer, 2008), flood forecasting (Wu et al., 2020), and climate studies (Mu et al., 2017; Parker, 2010). Ensemble models have gained momentum in large-scale water quality studies (Van Vliet et al., 2019), but their adoption in limnology has been slow. We believe the limnology community recognises the benefits of using ensembles and multi-model simulations (Nielsen et al., 2014; Stepanenko et al., 2010), but lacks scientific software to facilitate lake ensemble modelling. Past efforts to apply multiple lake models to the same study systems (Nielsen et al., 2014; Trolle et al., 2014; Yao et al., 2014; ISIMIP: Frieler et al., 2017; Gal et al., 2020; Kobler and Schmid, 2019; LakeMIP: Stepanenko et al., 2010) have often been the result of large international collaborations. While these initiatives have revealed pertinent new information, the labour required to build these networks is a barrier to broader implementation.

To remove these barriers and facilitate running ensembles of lake models, we developed LakeEnsemblR. Here, we describe the package version 1.0.0 and apply it to predict temperature and ice cover in two lakes. LakeEnsemblR is a numerical framework to run five 1D hydrodynamic lake models simultaneously (see Supplement - Table C1), using the same configuration and driver data, in the form of a package in the R software environment (R Core Team, 2020). The model source codes are open-source and the model executables can be run on Windows, MacOS, and Linux platforms. The two main objectives of LakeEnsemblR are a) to improve the accessibility of different hydrodynamic models for new users and b) to allow experienced users to utilise the powerful approach of running an ensemble of lake models in a consistent and coherent framework. These two aims are achieved through six key aspects of its functionality: 1) facilitating easy setup and configuration of model files; 2) running all models with standardised input files; 3) standardising model output; 4) providing tools for convenient post-processing; 5) standardising calibration routines; and 6) aggregating and enabling for ensemble averaging to account for different sources of uncertainty between the models. The structure of the package allows future development and addition of more models, and the code is freely accessible under a GNU General Public License v2.0.

2. Methods

2.1. Model descriptions

2.1.1. FLake

FLake (Freshwater Lake model, see Supplement -Table C1) is a bulk model that was developed primarily for fast lake-to-atmosphere coupling within numerical weather prediction models (Mironov, 2008, 2005). FLake simulates lake systems using a two-layer parametric representation focusing on the heat budget. The upper, well-mixed layer is considered thermally homogeneous, whereas the temperature in the lower, stably stratified layer is approximated by a self-similar (dimensionless shape) profile. FLake also uses self-similarity to model ice and sediment temperatures. Due to its computational efficiency, FLake has been widely used in numerical weather prediction models (Mironov et al., 2010; Šeparović et al., 2013) and lake studies on both global and local scale (Thiery et al., 2014 ; Vörös et al., 2010; Woolway et al., 2019). LakeEnsemblR version 1.0.0 uses a version of FLake that has been adapted to include heat input through inflows (pers. comm. Georgiy Kirillin). The default FLake model option implemented in LakeEnsemblR simulates the vertical temperature dynamics up to the mean depth of the lake, as FLake assumes a rectangular shape of the basin and does not incorporate the lake's specific hypsography. The assumptions of FLake match best when using the mean depth of the lake, therefore the FLake simulations extend to a shallower depth than the other hydrodynamic models.

2.1.2. GLM

The General Lake Model (GLM, see Supplement -Table C1) is a vertical 1D hydrodynamic lake model developed by the University of Western Australia (Hipsey et al., 2019). GLM applies a flexible Lagrangian structure to replicate mixing dynamics. Here, neighboring layers either split or merge depending on the density of the layers. Surface mixing dynamics are calculated via an energy balance approach, where the available kinetic energy is compared to the potential energy of the water column. The model has been widely applied, for example to simulate seasonal dynamics of temperature and ice cover (Bueche et al., 2017, Fenocchi et al., 2018), project impacts of water management measures on lake ecosystems (Feldbauer et al., 2020, Ladwig et al., 2018, Weber et al., 2017), and to assess scenarios regarding extreme events (Mi et al., 2018, Soares et al., 2019). It has also been rigorously tested in a large number of lakes (Bruce et al., 2018). In the version 1.0.0 of LakeEnsemblR, version 3.1.0 of GLM is used.

2.1.3. GOTM

The General Ocean Turbulence model (GOTM, see Supplement - Table C1) was developed by Burchard et al. (1999). It is a vertical 1D hydrodynamic water column model that includes important hydrodynamic and thermodynamic processes related to vertical mixing in natural waters (Umlauf et al., 2005). It was initially developed for modelling turbulence in the ocean (Burchard et al., 2006), but it has been adapted for use in hydrodynamic modelling in lakes (Sachse et al., 2014). GOTM has been used to model the dissolution of CO2 in lakes (Enstad et al., 2008), extreme events in a eutrophic marine system (Ciglenečki et al., 2015), impact of macrophytes on water quality (Sachse et al., 2014) and hindcasting and future climate change projections of the thermal structure of a lake (Ayala et al., 2020, Moras et al., 2019). LakeEnsemblR version 1.0.0 uses version 5.4.0 of the lake branch of GOTM.

2.1.4. Simstrat

Simstrat is a vertical 1D hydrodynamic lake model (see Supplement -Table C1), combining a buoyancy-extended k-epsilon model with seiche parameterisation, and was originally developed by Goudsmit et al. (2002). Simulated variables include surface energy fluxes, and vertical profiles of turbulent diffusivity and water temperature. Multiple options for external forcing are available, as well as variable wind drag coefficients, inflow settings, and ice and snow formation (Gaudard et al., 2019). Simstrat has been successfully applied in lakes and reservoirs of varying morphometry in different climate zones, and in scenarios regarding climate warming (Kobler and Schmid, 2019; Schwefel et al., 2016; Stepanenko et al., 2013; Thiery et al., 2014). The model is currently maintained by the "Surface Waters - Research and Management" Department of EAWAG (Switzerland) and version 2.4.1 is currently used in LakeEnsemblR.

2.1.5. MyLake

MyLake (Multi-year Lake simulation model, see Supplement - Table C1) is a vertical 1D lake model developed and hosted by the Norwegian Institute for Water Research (NIVA), the University of Helsinki (Finland), and Université Laval (Canada) (Saloranta and Andersen, 2007). MyLake simulates daily vertical profiles of lake water temperature, density stratification, seasonal ice and snow cover, sediment-water dynamics, and phosphorus-phytoplankton interactions (Saloranta and Andersen, 2007). The model has been used to simulate water temperature, ice and phytoplankton dynamics in mostly Northern and alpine regions (Couture et al., 2018; Kobler and Schmid, 2019; Saloranta et al., 2009). The version used in LakeEnsemblR version 1.0.0 is written in R and corresponds to the MyLake Matlab version 1.2.

2.2. R package description

R is an open-source and freely available statistical program that is widely used in the limnological community and has previously been used for community-developed tools, such as rLakeAnalyzer (Read et al., 2011; Winslow et al., 2019) and LakeMetabolizer (Winslow et al., 2016). All core functions in LakeEnsemblR version 1.0.0 have associated documentation with replicable examples all of which can be accessed through help functions within R (tested with versions 3.6.2 and 4.0.2, R Core Team, 2020).

2.2.1. Main workflow

The package works with one centralised configuration file, in which the user defines the settings of the model run and provides the locations of the standardised input files (see Box 1). The package exports the settings in the configuration file and the standardised input files to the requirements of each individual model (*export_config()* function), after which the models can be run (*run_ensemble()* function). The resulting water temperatures, densities, and ice cover thickness of the individual models are then compiled into a netcdf file and can be extracted or plotted in R (Fig. 1). If observations are provided, these are added to the netcdf file as well. Optionally, this process can be repeated with different forcing files or different parameter sets, to add multiple ensemble members to the netcdf (*run_ensemble()* function*, add=TRUE* argument*)*. This supports multi-model ensembles as well as simulations of multiple parameterisations of the same model(s). The combined model output can either be stored in text or netcdf format. In case observations are provided, parameter values of the different models can be calibrated (*cali_ensemble()* function), see section "Calibration algorithms" (Fig. 1).

2.2.2. Data requirements

The minimum data requirements to run LakeEnsemblR are a hypsographic file, a light extinction coefficient, an initial temperature profile, and a time-series of meteorological forcing variables. In the LakeEnsemblR configuration file, the user needs to provide the location of the files. The files should have specific headings, so the program can identify what information is provided (see **Supplement A**).

In the hypsographic file, the surface area (m^2) per depth (m) of the lake is given. The light extinction coefficient (m^{-1}) can be either given as a single value or varying over time. An initial temperature profile is needed if temperature observations are not provided for the simulation starting date. The meteorological forcing must have a constant time step and not contain missing values. Required meteorological forcing data include air temperature (°C) and downwelling shortwave radiation (W/m^2). Wind speed (m/s) needs to be given as well, either as a scalar or a vector (including wind direction). Either relative humidity (%) or dewpoint temperature (°C) needs to be provided, and if relative humidity is not provided, it is calculated from dewpoint temperature and air temperature according to the weathermetrics package (Anderson et al., 2013). Downwelling longwave radiation (W/m^2) can either be provided directly to the models, or if it is not, will be calculated internally from cloud cover (−), air temperature (°C), and humidity (relative humidity or dewpoint temperature), according to Konzelmann et al. (1994). Air pressure at lake surface level is also needed to run the models, but air pressure at sea level can be provided instead, in which case air pressure at lake surface level is estimated using the barometric formula, assuming a sea level temperature of 15 °C (Berberan-Santos et al., 1997). Lastly, providing precipitation (mm/h or mm/d) is optional, but omitting it will cause the models that require precipitation (GOTM and GLM) to be run with a precipitation of 0, which may result in issues with the water balance. The influence of direct precipitation on the heat budget tends to be minimal (Imboden and Wüest, 1995).

Optional data that can be provided are discharge (m^3/s), temperature (°C) and salinity (PSU) of inflows, as well as water temperature and ice thickness observations. In the present version of LakeEnsemblR, outflow discharges can only be set to be identical to inflows, due to the many differences between the models in water balance calculations. Varying water levels are therefore not yet supported, although users can change model-specific settings related to the water balance. Observations are used for initialising temperature profiles, calibration, and plotting. If provided, observations are added to the output netcdf file.

2.2.3. Getting started

The LakeEnsemblR code is available on GitHub (https://github.com/aemon-j/LakeEnsemblR) and needs to be installed into the R environment, following instructions on the GitHub page. LakeEnsemblR itself cannot run the models, but instead this is done through supporting

Box 1
Settings controlled by the LakeEnsemblR configuration file. Whenever it is stated "Link to … file", the file path to the LakeEnsemblR standardised file should be given. The configuration file is written in yaml text format and is easily readable in any text editor. Comments are provided in the example configuration file to explain what each parameter does and what the input options are.

- Location
  - Coordinates
  - Elevation
  - Depth
  - Hypsograph
- Time
  - Start and end date of simulation
  - Model integration time step
- Config files
  - Links to model-specific configuration files
- Observations
  - Links to observational data (water temperature, ice thickness)
- Input
  - Link to meteorological forcing
  - Link to initial temperature profile
  - Light extinction coefficient (constant or varying over time)
  - Switch ice models on or off
- Inflows
  - Switch on or off
  - Link to inflow file
- Output settings
  - File format
  - Depth resolution
  - Output time step
  - Variables to generate output for
- Meteorological scaling factors (optional)
- Model-specific parameter values
  - In this section, the user can change values in the model-specific configuration files
- Calibration settings
  - Initial value, lower and upper boundaries for calibration of either model-specific parameters or scaling factors for the meteorological forcing.

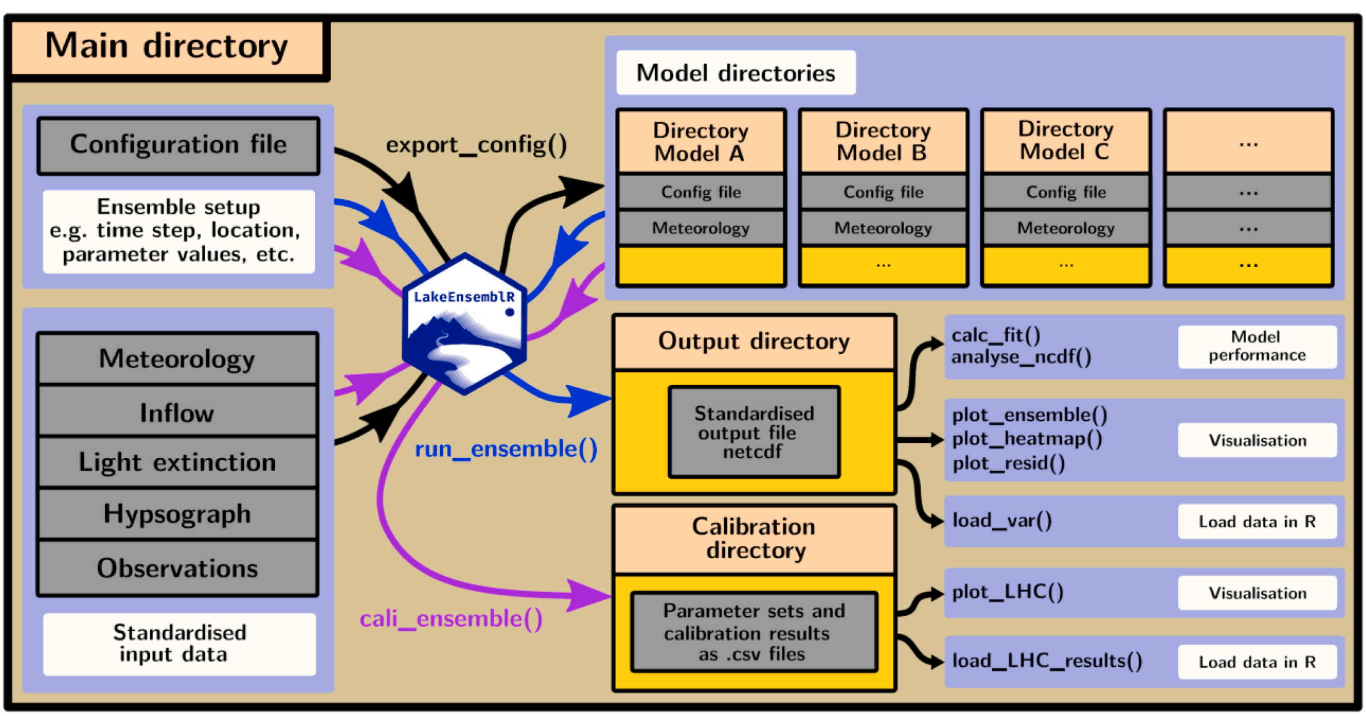

Fig. 1. Conceptual overview of the LakeEnsemblR package showing the main folder structure and important functions.

R packages (FLakeR, GLM3r, GOTMr, SimstratR, MyLakeR), which contain ways of running each model on the platforms Windows, MacOS, or Linux, through executables contained in the packages or having the model code in R.

After LakeEnsemblR is installed, a folder containing the setup for the ensemble run should be created. This can be done by editing the template folder provided within the package or by copying a setup from https://github.com/aemon-j/LER_examples. The LakeEnsemblR configuration file (in yaml format) contains all modifiable settings and input file paths. The input files themselves (e.g. for meteorology or inflows) need to be in comma-delimited format and need to have the correct column headers. Templates for any file can be generated through the *get_template()* function. Once the configuration file and the input files have been set up, the *export_config()* function can be run. This function exports the settings in the LakeEnsemblR configuration file and the LakeEnsemblR input files as required by each individual model. This means that for some models, units are converted, model parameters are changed, or input files are saved in a different format. The setup for each individual model is placed in its own directory.

After running *export_config()*, the ensemble can be run through the *run_ensemble()* function. In each model folder, the model-specific output is generated, which is then written to a netcdf file or text files (user choice) in a shared "output" folder. *run_ensemble()* runs the models without calibration. The *cali_ensemble()* function runs the calibration, following the specifications in the calibration section of the LakeEnsemblR configuration file, and stores the results of the calibration in the folder specified by the *out_f* argument. If netcdf output is chosen, several functions are available in the package to visualise the output (*plot_heatmap()*, *plot_ensemble()*, *plot_resid()*), load the data into R (*load_var()*), determine start and end of stratification and ice cover (*analyse_ncdf()*), or calculate goodness-of-fit (*calc_fit()*). Each function has documentation that can be loaded in R by typing *?name_function*.

While the running and calibration of the models is controlled by the R code, both the input and output files are in formats that are accessible by a wide array of software. Therefore, it is possible for users to do the pre- and post-processing with different software. A vignette is available on the LakeEnsemblR GitHub repository, which describes step-by-step how to run an ensemble, with multiple code examples. A wiki is available with additional information and frequently asked questions.

2.2.4. Calibration algorithms

The LakeEnsemblR package provides functionality for automated parameter estimation using one of three methods. A simple calibration method based on Latin hypercube sampling, a Markov Chain Monte Carlo approach (MCMC), and a method for constrained fitting of the models to data using one of several available standard optimisation algorithms. The last two methods are implementations of the R package FME (Soetaert and Petzoldt, 2010) using the functions *modMCMC()* and *modFit()*, respectively. Details about the MCMC and constrained fitting can be obtained from Soetaert and Petzoldt (2010) and the sources given therein. The Latin hypercube sampling method uses upper and lower bounds for all parameters that are to be calibrated and then samples evenly within the parameter space given by these bounds (e.g., Mckay et al., 2000). Then the models are run and evaluated for all sampled parameters sets. By default, six measures of model performance are calculated: root mean square error (RMSE), Nash–Sutcliffe efficiency (NSE), Pearson correlation coefficient (r), mean error (bias), mean absolute error (MAE), and normalised mean absolute error (NMAE) (see Table C2 in the supplement). The user can also supply their own quality function which calculates measures of fit from modeled and observed data. Each of the three calibration methods can be run in parallel computation, where the models are distributed over the available cores. The parameters which are to be estimated, and their upper and lower bounds (if applicable) are specified in the master configuration file.

Scaling factors of meteorological forcing are parameters that are often calibrated in models (e.g., Ayala et al., 2020; Gaudard et al., 2019). Some models within LakeEnsemblR have internal parameters that scale the (meteorological) forcing, but not all. In order to be able to use the same scaling factors for all five models, the calibration section of the master configuration file distinguishes between model-specific parameters and meteorological (scaling) parameters. All three calibration methods can be used to obtain parameters that optimise the chosen model performance measure for the individual models. If common optimum scaling factors for all models in the ensemble are wanted, the user needs to apply their own method to aggregate the scaling factors of the models.

2.2.5. Combining multiple ensemble runs

Uncertainty of lake model output comes from different sources that are related to: forcing data, initial conditions, model parameter values, or structural reasons like process description and numerical methods (Thomas et al., 2020). LakeEnsemblR foremost tackles the uncertainties related to structural differences between different models. But, LakeEnsemblR can also be used to address other sources of uncertainties; the *run_ensemble()* function allows to add different model runs to a single netcdf file. Using this functionality, model runs with different parameterisations, forcing data, or initial conditions can be run and compared. Many diagnostic functions like *calc_fit()* or *plot_ensemble()* have two additional arguments *dim* and *dim_index* to select which dimension should be used.

3. Example application of LakeEnsemblR

We applied the LakeEnsemblR package to two lake case studies: Lough Feeagh (IE) and Langtjern (NO). Lough Feeagh is a temperate monomictic lake with a maximum depth of 46 m and a surface area of 3.9 km^2. Langtjern is a shallow dimictic lake with a maximum depth of 12 m and a surface area of 0.23 km^2. Langtjern is separated into three distinct basins and our modelling efforts concentrated in the north basin with a maximum depth of 9 m and surface area of 0.06 km^2. A detailed description of Lough Feeagh can be found in Allott et al. (2005), or de Eyto et al. (2016), and a detailed description of Langtjern can be found in Couture et al. (2015); Henriksen and Wright (1977); Wright (1983).

The Latin hypercube sampling method with 500 parameter sets was applied to both study cases. For each model, the parameter set with the lowest RMSE was selected. One full year was used to calibrate the models (2013 for Lough Feeagh, May 2014 to May 2015 for Langtjern), and the following year was reserved for validation of the simulated temperatures. Scaling factors for wind speed and shortwave radiation were calibrated for all five models, and in addition model-specific parameters *k_min* (GOTM), *coef_mix_hyp* (GLM), *c_relax_C* (FLake), *a_seiche* (Simstrat), and *C_shelter* (MyLake) were calibrated as well. These parameters were selected from parameters used for calibration in previous studies (see Supplement - Table C3). The inflows and outflows were omitted in all simulations. For the Langtjern simulation, hourly meteorological forcing was used to explore water temperature and ice dynamics, whereas for Lough Feeagh, the models were calibrated and validated using both hourly and daily averaged values to compare performance of water temperature, except for MyLake which only operates at the daily time scale.

In this section, we provide an example of how LakeEnsemblR can be used to partition and quantify different sources of uncertainty; boundary conditions, initial conditions, parameter and structure uncertainty. In order to do this, the Lough Feeagh ensemble was run a total of 300 times over a period of 16 days during the stratified period (June 12th to June 27th, 2013), while different factors were varied to estimate their impact on the simulation output. To isolate the effect of initial conditions, the models were run using 100 different initial temperature profiles, that were drawn from a normal distribution around the observed value with a standard deviation of 0.1 °C. For boundary conditions the models were forced with 100 different versions of the meteorological data, where random noise was added to air temperature and wind speed from normal distributions with a mean of 0 °C and a standard deviation of 0.5 °C, and a mean of 0 m/s and a standard deviation of 0.5 m/s, respectively. For parameter uncertainty, 100 parameter values were drawn for each calibrated parameter using either a normal or lognormal distribution (Table C4). To quantify and compare the variation of the different model runs between the different sources of uncertainty, the standard deviation of the water temperature for each time step at two depths (0.9 m and 16 m) of the output was calculated across the 100 ensembles, for each model separately.

For Lough Feeagh, we additionally ran an ensemble with different parameterisation of the five models to compare the uncertainty related to the chosen model with the uncertainty related to the calibrated parameters and scaling factors for each individual model. Starting from the Latin hypercube calibration (using daily forcing data), we first selected the best 10% parameter sets in terms of their RMSE for each model. From these sets, we extracted the range of the calibrated parameter and scaling factors and then sampled 20 parameter sets for each model within this range using Latin hypercube sampling. Then we ran the ensemble using these parameter sets and combined all ensemble runs in one netcdf file.

3.1. Lough Feeagh: water temperature dynamics

Both simulations in Lough Feeagh using daily and hourly meteorological forcing generally produced satisfactory results of simulated temperature in the calibration period, compared to other simulations (e.g. Arhonditsis et al., 2006; or Arhonditsis and Brett, 2004), with RMSE <1.3 °C for daily forcing (Table 1, Fig. 2) and RMSE < 0.9 °C for hourly forcing (Table 2). Except for FLake, even the uncalibrated model runs had satisfactory model performance, and calibration improved the model fits further. Compared to the calibration period, most models performed worse during the validation period (Table 1 for daily data and Table 2 for hourly data). Except for Simstrat, during the calibration phase all models tended to underestimate water temperatures over all depths and throughout the year (Fig. 3), on average ranging from about 0.1 °C (GLM, hourly forcing, Tables 2)–1 °C (GOTM, daily forcing, Table 1).

In general, the calibrated model performance was better using hourly forcing data compared to daily forcing data. Of the five models, FLake performed poorest when using daily forcing data and GLM performed poorest when using hourly forcing data. The best performing model differed between hourly and daily forcing data with GOTM performing best when using hourly data (calibration phase), and Simstrat performing best when using daily data (calibration and validation phase). In all models the largest residuals were seen at observed temperatures of 10–15 °C, during the time of the onset and end of summer stratification, and around the depth of the thermocline (Fig. 3). Using daily average forcing data, the ensemble average was amongst the best performing fits and when using hourly forcing data the ensemble mean outperformed the individual models in most of the calculated performance measures, due to errors of individual models cancelling each other out in the ensemble mean (Tables 1 and 2).

3.2. Langtjern: lake ice dynamics

The models FLake, GOTM, MyLake and Simstrat accurately captured the onset of ice cover on Langtjern (−5 to +9 days) while GLM had larger errors (+10 to +17 days) (Fig. 4). The ensemble mean, which was calculated by taking the average of the day of year when ice onset and ice-off occurred, was also relatively accurate (+3 to +6 days). For capturing the disappearance of ice cover, there was larger variability between the models compared to ice onset. In both years, GOTM and Simstrat predicted ice-off too early (−44 to −16 days). GLM overestimated ice-off in 2015 and 2016 by 27 to 19 days, respectively, whereas FLake and MyLake predicted ice-off relatively accurately both years (−1 to +8 days).

The temperature profiles had a larger RMSE for the calibration and validation period in general for Langtjern compared to Lough Feeagh, particularly MyLake (3.62–4.24 °C) and GOTM (3.36–4.70 °C) (Table 3). These models failed to accurately simulate the stratification structure with increased mixing during the summer months leading to larger errors. FLake had the lowest uncalibrated RMSE (2.02 °C), which was further reduced following calibration (1.08 °C). For summary plots of Langtjern of the model ensemble and residuals see Figure B1 and **B2**.

3.3. Uncertainty partitioning

Parameter uncertainty had the largest effect on the standard deviation of water temperatures at the depth of 0.9 m compared to initial conditions and boundary conditions for all the models except FLake in Lough Feeagh (Fig. 5). Each of the parameters chosen were to account for mixing within the water column but their implementation in each model is different due to the different formulation of mixing equations in each model. Also, the distributions of these parameters were not

Table 1

Model results or goodness-of-fit - uncal(ibrated), cal(ibrated), and val(idated) - for water temperature (°C) in Lough Feeagh using daily forcing data. Calibration was done for the year 2013 and validation for the year 2014. The best model performances are marked in bold. Shown are Root Mean Square Error (RMSE), Pearson's r (r), Nash-Sutcliffe Efficiency (NSE), Normalised Mean Absolute Error (NMAE), Mean Absolute Error (MAE), and Bias (or mean error).

measure	period	FLake	GLM	GOTM	Simstrat	MyLake	Ensemble mean
RMSE	uncal	3.057	0.846	1.698	**0.625**	1.719	1.189
	Cal	1.210	0.670	1.261	**0.502**	0.656	0.629
	Val	2.297	0.847	1.425	**0.693**	0.780	0.916
r	uncal	0.682	**0.979**	0.965	0.977	0.946	0.974
	Cal	0.804	0.983	0.969	0.983	0.983	**0.985**
	Val	0.756	0.981	0.964	0.986	**0.988**	0.984
NSE	uncal	0.631	0.948	0.788	**0.971**	0.783	0.896
	cal	0.942	0.967	0.883	**0.982**	0.968	0.971
	val	0.776	0.944	0.840	**0.962**	0.952	0.934
NMAE	uncal	0.175	0.082	0.165	**0.044**	0.131	0.101
	cal	0.072	0.070	0.133	**0.035**	0.065	0.064
	val	0.132	0.081	0.132	**0.045**	0.067	0.079
MAE	uncal	2.011	0.691	1.501	**0.438**	1.318	0.962
	cal	0.812	0.558	1.152	**0.337**	0.533	0.534
	val	1.610	0.720	1.286	**0.467**	0.628	0.760
Bias	uncal	−1.909	−0.575	−1.484	**0.038**	−1.308	−0.955
	cal	−0.720	−0.347	−0.986	**0.028**	−0.436	−0.458
	val	−1.560	−0.362	−1.048	**−0.352**	−0.526	−0.664

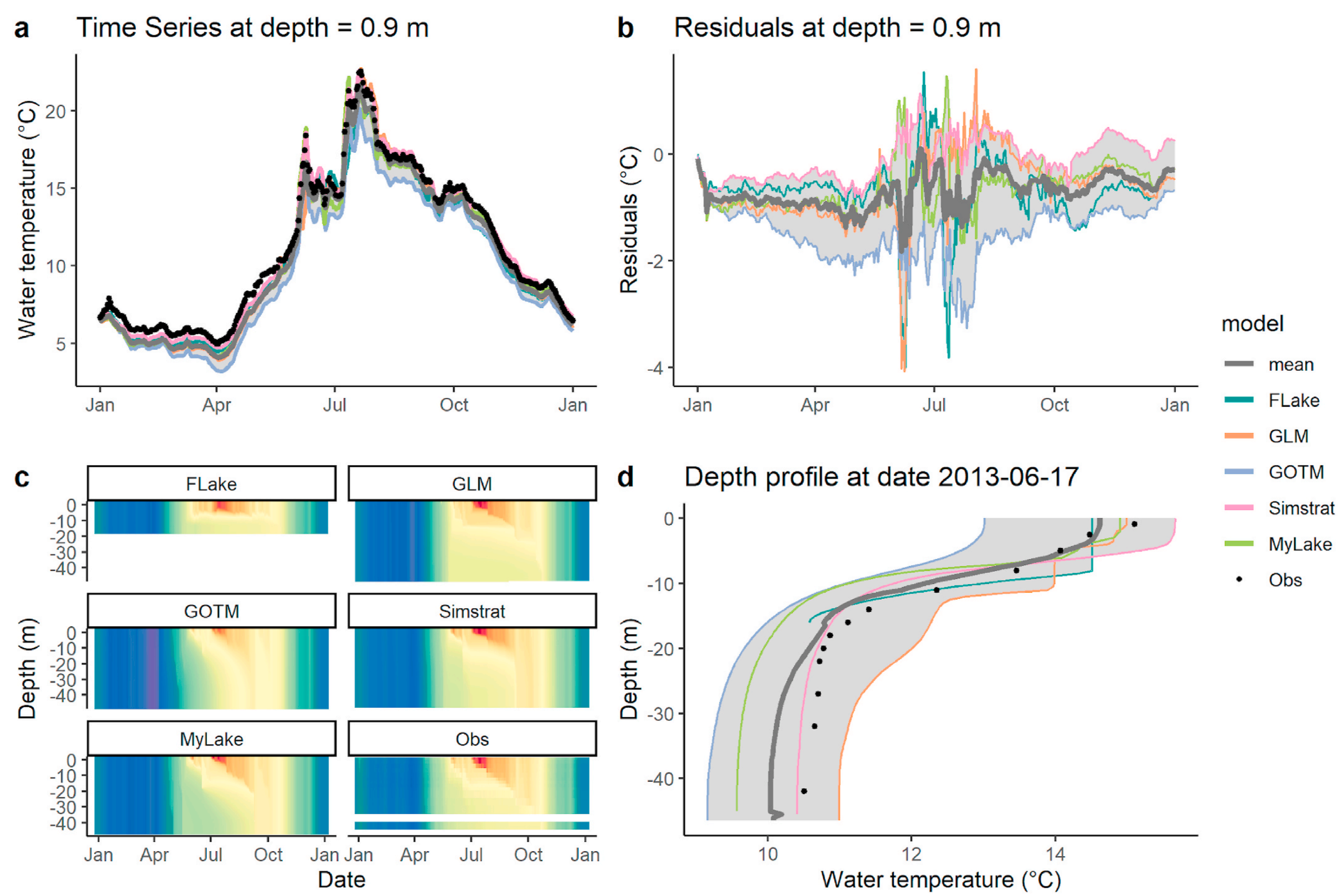

Fig. 2. Calibrated ensemble output for simulated water temperature in 2013 for Lough Feeagh using daily forcing data, showing: **a** time series of model output at 0.9 m depth for all models, **b** residuals for the time series at 0.9 m depth, **c** filled contour maps from each of the models and observations, and **d** the ensemble modeled depth profile for 17 June 2013.

Table 2
Model results or goodness-of-fit - uncal(ibrated), cal(ibrated), and val(idated) - for water temperature (°C) in Lough Feeagh using hourly forcing data. MyLake cannot be run with hourly time steps and was therefore not included in this table. Calibration was done for the year 2013 and validation for the year 2014. The best model performances are marked in bold. Shown are Root Mean Square Error (RMSE), Pearson's r (r), Nash-Sutcliffe Efficiency (NSE), Normalised Mean Absolute Error (NMAE), Mean Absolute Error (MAE), and Bias (or mean error).

measure	period	FLake	GLM	GOTM	Simstrat	Ensemble mean
RMSE	Uncal	2.957	0.943	0.801	1.107	**0.726**
	Cal	0.617	0.819	0.594	0.599	**0.469**
	Val	0.607	1.174	0.855	0.701	**0.570**
r	Uncal	0.682	0.971	**0.977**	0.966	0.976
	cal	0.816	0.977	0.983	0.979	**0.985**
	val	0.824	0.972	0.984	0.985	**0.992**
NSE	uncal	0.655	0.935	0.953	0.910	**0.961**
	cal	**0.985**	0.951	0.974	0.974	0.984
	val	**0.984**	0.891	0.942	0.961	0.974
NMAE	uncal	0.157	0.081	0.074	0.072	**0.063**
	cal	**0.040**	0.066	0.058	0.046	0.045
	val	**0.044**	0.087	0.070	0.047	0.051
MAE	uncal	1.909	0.718	0.634	0.756	**0.581**
	cal	0.413	0.600	0.477	0.445	**0.378**
	val	**0.461**	0.874	0.672	0.496	0.466
Bias	uncal	−1.749	−0.340	−0.489	0.567	**−0.305**
	cal	−0.191	**−0.091**	−0.318	0.074	−0.126
	val	−0.300	**0.096**	−0.548	−0.345	−0.272

comparable between models with some being normally distributed while others were log-normal distributed (Table C4). As such, parameter-uncertainty cannot accurately be compared between models, but it can be accounted for when using a one-model ensemble. Across the different models, boundary conditions were more sensitive for GLM than for the other models, at both 0.9 m and 16 m depth. With regards to uncertainty in the initial conditions, FLake and GLM had higher standard deviation at 0.9 m compared with GOTM, Simstrat and MyLake. GLM had a much higher standard deviation at 16 m for initial conditions, boundary conditions and parameter uncertainty. This is partly due to the strong stratification which is seen in GLM (Figure B3). For parameter uncertainty, GOTM, Simstrat and GLM had a high standard deviation at 0.9 m and 16 m, while it was lower for MyLake and FLake had the lowest uncertainty. s.

3.4. Multi-parameter ensemble

The model-specific parameters and scaling factors that resulted in good model performance had a broad distribution (see Figure B4 in the Supplement as an example). For the model-specific parameters of FLake, GLM, and Simstrat as well as for the shortwave radiation scaling factor for FLake and Simstrat this distribution spanned more than 75% of the range given in the calibration process. This suggests that the chosen parameters are interrelated and there might not be a single best parameter set, that the parameters were non-sensitive, or that the parameter range in the calibration was too narrow. The application of a multi-parameter ensemble is showing the uncertainty related to not being able to clearly identify a single best parameter set (Fig. 6). The

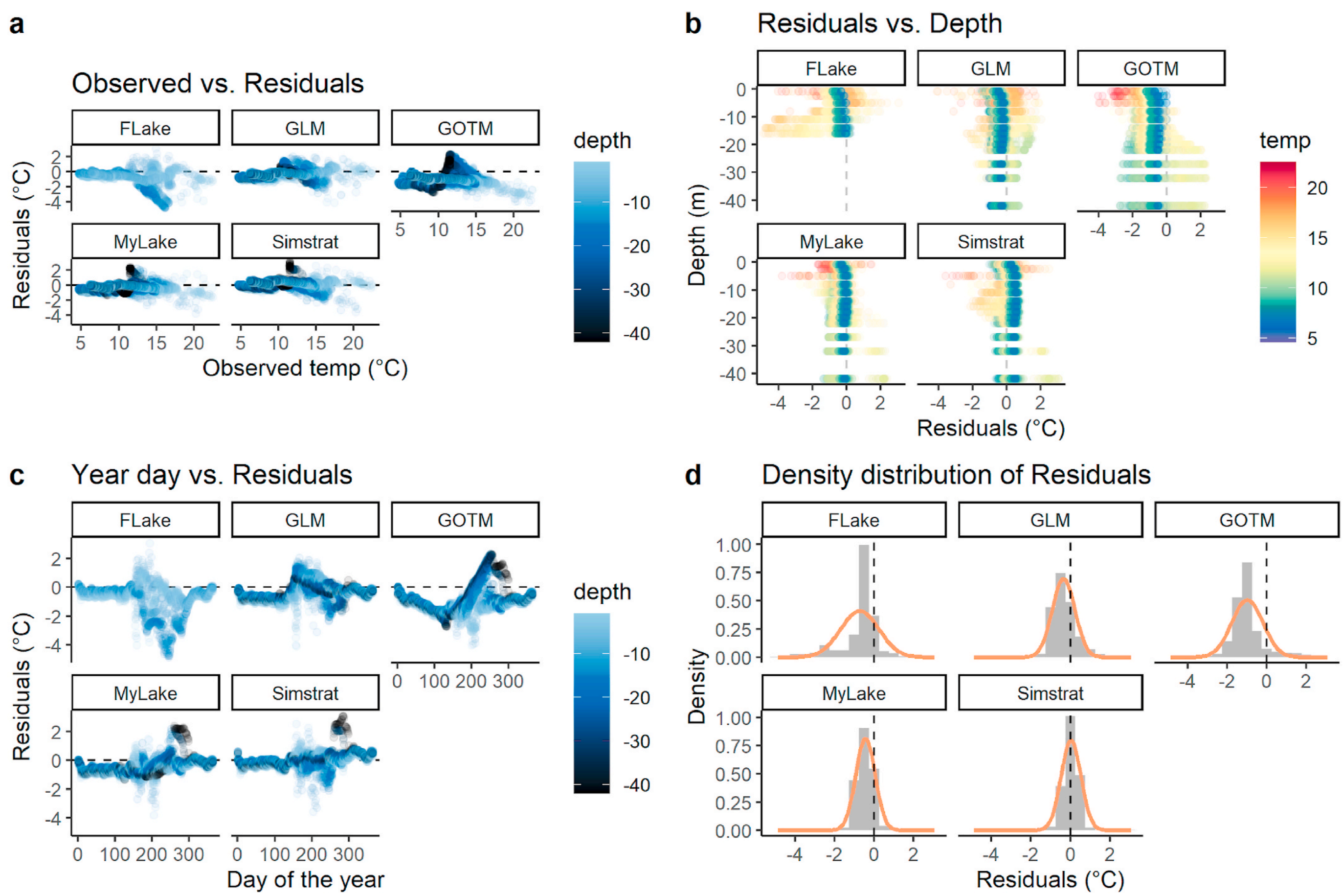

Fig. 3. Water temperature residual diagnostic outputs from the calibrated ensemble run for Lough Feeagh in the year 2013 using daily forcing data. **a** Observed water temperature vs. residuals; **b** residuals vs depth, with the absolute simulated temperature in °C; **c** day of the year vs residuals and **d** distribution of the residuals.

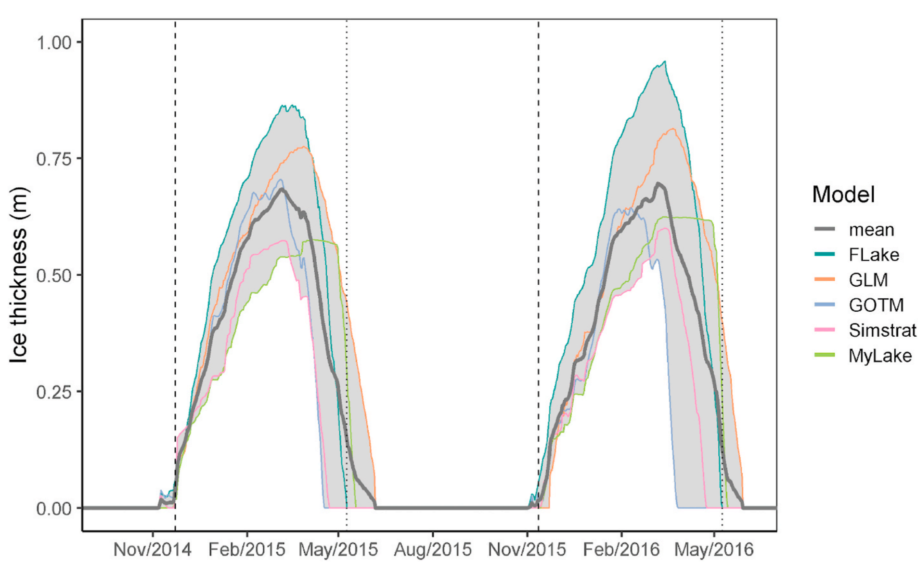

Fig. 4. Calibrated ensemble model time series output for ice thickness for Langtjern, Norway. Dashed lines indicate the observed onset of ice and dotted lines indicate observed ice-off.

uncertainty of the simulated water temperature was larger during summer months and at greater depths for all models. For the water temperature close to the surface (0.9 m depth) the uncertainty due to the chosen model was slightly larger than the one related to the calibrated parameters throughout the year, for all models. At 16 m depth the uncertainty due to the calibrated parameter was about the same as the one related to the used model.

Table 3
Model results or goodness-of-fit - uncal(ibrated), cal(ibrated), and val(idated) - for water temperature (°C) in Langtjern using hourly forcing data (as MyLake requires daily input, LakeEnsemblR averages sub-daily input to daily time steps for MyLake simulations). Calibration was done for the year 2014–15 and validation for the year 2015–16. The best model performances are marked in bold. Shown are Root Mean Square Error (RMSE), Pearson's r (r), Nash-Sutcliffe Efficiency (NSE), Normalised Mean Absolute Error (NMAE), Mean Absolute Error (MAE), and Bias (or mean error).

Measure	Period	FLake	GLM	GOTM	Simstrat	MyLake	Ensemble Mean
RMSE	uncal	**2.020**	2.394	4.696	3.437	4.416	2.838
	cal	**1.084**	2.164	3.364	2.568	3.626	3.013
	val	**1.135**	1.764	4.045	4.171	4.242	3.699
r	uncal	**0.887**	0.868	0.786	0.833	0.807	0.874
	cal	**0.983**	0.906	0.865	0.913	0.845	0.881
	val	**0.983**	0.938	0.818	0.755	0.786	0.824
NSE	uncal	**0.895**	0.760	0.074	0.504	0.181	0.662
	cal	**0.963**	0.794	0.501	0.709	0.420	0.622
	val	**0.962**	0.862	0.275	0.229	0.203	0.433
NMAE	uncal	**0.453**	0.530	0.910	0.632	0.659	0.492
	cal	0.450	**0.433**	0.817	0.569	0.599	0.587
	val	0.454	**0.362**	0.828	0.677	0.636	0.602
MAE	uncal	**1.260**	1.601	3.515	2.637	3.126	1.929
	cal	**0.830**	1.469	2.686	2.211	2.818	2.189
	val	**0.863**	1.022	3.017	3.059	2.880	2.361
Bias	uncal	0.985	**−0.298**	1.076	−0.515	0.409	0.344
	cal	0.274	−0.575	0.313	−0.834	−0.615	**0.019**
	val	0.399	**−0.104**	0.823	−1.062	0.160	0.328

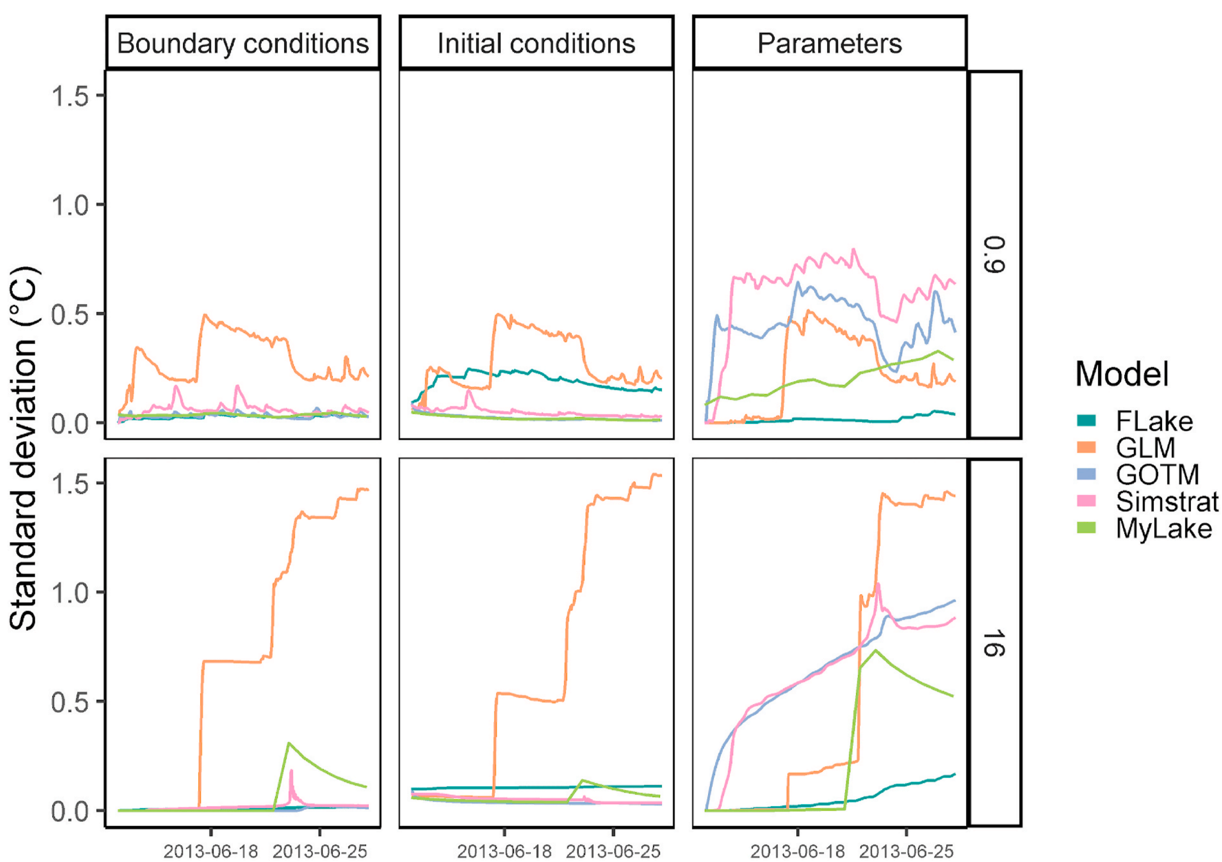

Fig. 5. Partitioning of the different sources of uncertainty for ensemble simulations in Lough Feeagh; boundary conditions, initial conditions and parameters between models at depths of 0.9 m and 16 m. Each model was simulated 100 times for 16 days with adjustments to the boundary conditions, initial conditions, and model parameters accordingly. Standard deviation was calculated across all 100 simulations for each day.

3.5. Discussion

As the simulations with hourly time step in Lough Feeagh show, the ensemble mean can outperform individual lake models, which is in line with the findings of Trolle et al. (2014) and Kobler and Schmid (2019). For the Lough Feeagh simulations with a daily time step, the Simstrat model performed best, followed by the ensemble mean and MyLake. Using hourly time steps, GOTM performed best of the four models individually, albeit not as good as the ensemble mean. In Langtjern, FLake simulated water temperature profiles best, while Simstrat and

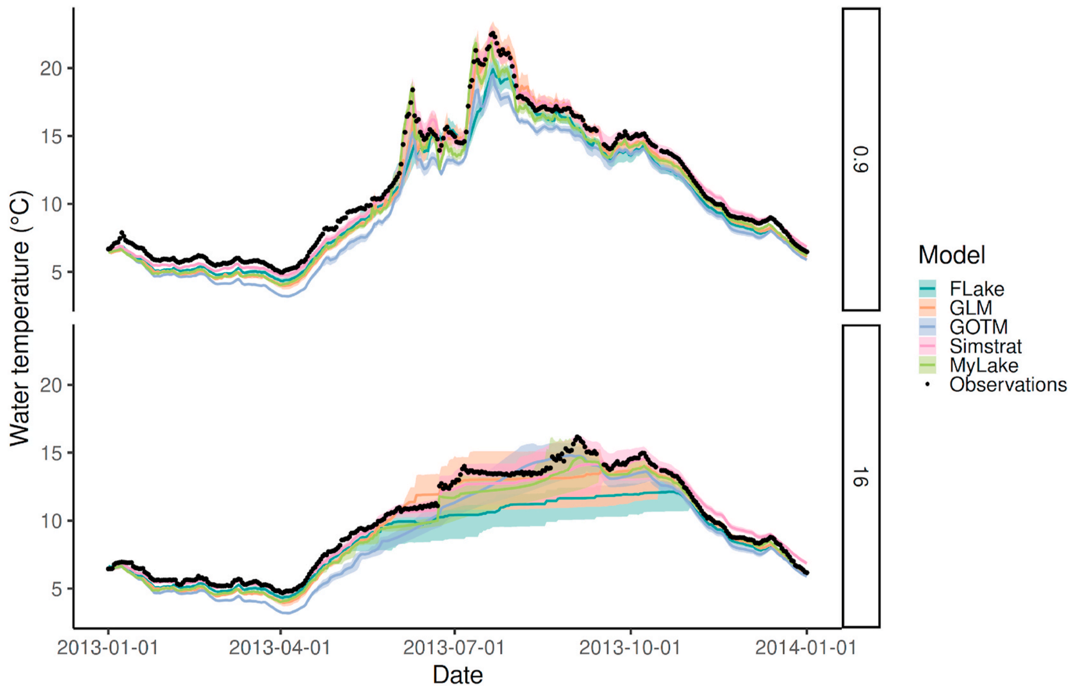

Fig. 6. Uncertainty of the simulated water temperature due to the calibrated model parameter and scaling factors for the five models in Lough Feeagh, at 0.9 m depth and 16 m depth. The shaded areas give the range of values of an ensemble of 20 model runs with different parameterisation.

MyLake performed the worst, although these two models simulated ice-on and ice-off well. In both Lough Feeagh and Langtjern, most models performed worse in the validation period than in the calibration period, which is to be expected due to the short (1 year) calibration period.

As shown in this study, and also observed while testing LakeEnsemblR in multiple other lakes (unpublished results), the best-performing model could vary per study case, and no single model consistently outperformed others. This shows an advantage of using ensembles compared to single model simulations, which are not likely to provide an optimal fit in every circumstance, while ensembles can incorporate individual strengths of multiple models. Similarly, ensemble modelling can highlight weaknesses of individual models compared to others which can further aid in model selection or refinement.

Ensemble predictions also give an indication of the uncertainty due to a different process description or parameterisation. This uncertainty may vary over depth or time (e.g. Figs. 2 and 5). An increased uncertainty in ensemble predictions represents diverging behaviour of different ensemble members. It might be important to interpret model predictions during periods with increased uncertainty with additional caution, and ensembles are a way to identify these periods. For a single set of parameters, the investigation of model-specific residuals in particular (e.g. Fig. 3) supports the quantification of uncertainty and the identification of better suited models for specific case studies. In the Lough Feeagh case study, the models GOTM, MyLake and Simstrat had a bias for simulated water temperatures near the lake bottom and during fall mixing (Fig. 3 a and 3 b). By looking at the depth-discrete residual dynamics (Fig. 3 c) as well as the density distribution of residuals (Fig. 3 d), the model with the lowest overall bias for Lough Feeagh was GLM (scattering over the whole vertical axis) and Simstrat (negative bias at surface and positive bias at bottom). Running a calibrated model ensemble allows the user to quantify these model-specific biases and uncertainties, making scenario projections or forecastings more robust. Additionally, running ensembles with different parameterisations, initial conditions, or different boundary conditions can help to quantify the uncertainties related to the respective source.

Similarly to Kobler and Schmid (2019) and Yao et al. (2014), there was large variation between the different models in predicting ice cover phenology (Fig. 4). However, most models captured the overall timing of ice-on and ice-off, which play a key role in the subsequent timing of stratification and several ecological processes in a lake. The ensemble represents the large uncertainty that is inherent in modelling lake ice cover (Sharma et al., 2019), which is important to account for when modelling lakes with periodic ice cover. It has recently been shown that the ensemble mean of ice timing and thickness can perform better than the individual models (Kobler and Schmid, 2019), which was supported here.

A key part of modeling is being able to identify and quantify the different sources of uncertainty. This is especially important if the model is to be used in a forecasting framework. Thomas et al. (2020) used a single one-dimensional hydrodynamic model and partitioned out the sources of uncertainty over a 16-day forecast of water temperature profiles in a reservoir. Using the LakeEnsemblR framework, this can be explored and quantified further, using multiple models. The brief examples that are shown in Figs. 5 and 6 are a way in which such an analysis can be conducted and the information gained from this exploration can inform decisions on model and parameter selection.

4. Summary

4.1. Framework

LakeEnsemblR facilitates the pre-processing of data that is needed to run multiple 1D models and combines the results into a single, standardised output file. Each model in the package requires a different format and structure of its configuration and input files. This has been standardised in LakeEnsemblR by requiring only one set of input and configuration files and by using the same format for all input files. By having to specify a specific header for each column of an input file, mistakes involving column order and units are avoided, and in the configuration file only a reference to the file location needs to be given, instead of having to specify which column contains what information.

LakeEnsemblR relies on R packages for each model, hosted on GitHub and archived in Zenodo (see Software Availability). These packages contain pre-compiled model executables for the platforms Windows, MacOS, and Linux, or the model code in R. This greatly facilitates user access to the models, as the ability to run the models is gained fully within the R environment. Some models provide pre-compiled executables on their respective websites, but often for only one platform, which regularly requires users to compile the model themselves. LakeEnsemblR removes this initial hurdle for modellers who want to apply one or multiple models.

The calibration methods provided in LakeEnsemblR can all be applied to the models without requiring the user to write custom calibration scripts. The ability to use the same calibration method for multiple models increases the comparability of the simulations. Results in the present study confirm that LakeEnsemblR's calibration methods can markedly improve model fit.

Like the input, each model generates its own specific output, often in different file types and consisting of different variables and units. LakeEnsemblR combines these outputs into one standardised format, either in text or netcdf. This allows quick application of the post-processing functions provided in LakeEnsemblR (e.g. *analyse_ncdf()* and *plot_heatmap()*), but also makes it easier for users to extract output and process the results in their preferred way. The standardised output is only generated for variables that are shared between the models. However, the full model-specific output is still available in the model output folders and can be accessed by the users.

By facilitating pre-processing, running, calibration, and post-processing, LakeEnsemblR supports accessible model ensemble applications by aquatic modellers new to the field. However, because all files required to run the models are present in the model folders, it in no way restricts more experienced users from using the full functionality of each of the different models. The "model parameters" section of the LakeEnsemblR configuration file allows the user to change any parameter in the model-specific configuration files, and files generated by LakeEnsemblR's *export_config()* function can be manually altered before starting the ensemble run.

4.2. Recommendations for use

LakeEnsemblR eases the configuration, running and processing of a hydrodynamic lake model ensemble, and allows the user to explore the results in various ways. However, by making it easier to apply multiple models, there is the risk that less attention will be paid to individual model setup and that models may be applied to situations beyond what they were designed and tested for. For example, by considering five models at once, the overall number of parameters increases markedly and the user might be tempted to only use default parameter settings without critical consideration of the consequences.

In order to properly calibrate a model and avoid problems such as nonuniqueness of calibrated parameter sets (i.e. equifinality - see Beven, 2006) it is important to make deliberate decisions and employ rigorous model validation. In addition to looking at single performance metrics for the simulated state variables, it is advisable to assess the model's capability to reproduce fluxes and emerging properties, patterns, and relationships (Hipsey et al., 2020). In order to find and select the right parameters to calibrate, the best practice approach would be to apply a sensitivity analysis (e.g. Andersen et al., 2021). Many methods for sensitivity analysis are available, but the Latin hypercube sampling method included in LakeEnsemblR can be used as an initial approach to quantify sensitivity. Where a complete sensitivity analysis is not feasible, expert or a priori knowledge on the models should be used to select the calibration parameters. In the present study, we aimed at demonstrating the possibility of calibration with LakeEnsemblR rather than exploring the parameter sensitivity of each model, and we chose model parameters based on the parameter selection done in previous studies (see Table C3 in the Supplement for parameters that were calibrated in previous studies).

However, the possibility to combine runs with multiple models and parameterisations also is an opportunity to tackle issues regarding sources of uncertainty. LakeEnsemblR can be used to quantify different sources of uncertainty (boundary conditions, initial conditions, parameter, model structure), increase understanding about what model works best under different circumstances, and also within-model comparisons can be made. Although not applied in the present study, post-processing techniques applied in other research fields, such as blending (Vannitsem et al., 2020), can be applied to the ensemble result so that ensemble members are weighted and more information is retrieved from the ensemble. However, we advocate the use of LakeEnsemblR within established modelling practices (e.g., Arhonditsis and Brett, 2004; Hipsey et al., 2020), rather than as a replacement.

4.3. Outlook

The simulations in Lough Feeagh and Langtjern showcase the main functionalities of the package. However, LakeEnsemblR can be applied to a wider range of locations and scenarios. In long-term climate simulations, lake model ensembles have been applied as part of the Inter-Sectoral Impact Model Intercomparison Project (ISIMIP) (Frieler et al., 2017; Vanderkelen et al., 2020), and LakeEnsemblR can facilitate similar efforts. Ensembles offer several possibilities for weekly or seasonal forecasting efforts (e.g.,Krishnamurti et al., 2000; Thomas et al., 2020), and LakeEnsemblR can be run not only with multiple models, but also forced with several different weather forecasts. Studies of processes in lake physics that are difficult to model, such as consequences of extreme weather events (Mesman et al., 2020) or lake ice phenology (Yao et al., 2014), can especially benefit from an ensemble approach. While LakeEnsemblR currently only covers hydrodynamic models, its predictions can also serve as input for water quality models. Such a water quality ensemble can ultimately serve to assess and qualify the performance of multiple aquatic ecosystem models (Hipsey et al., 2020), while also giving uncertainty to the ecological impacts of management scenarios on ecosystems. More applications are possible, and the modular structure of the LakeEnsemblR code allows for the addition of new models and continued development.

Although the advantages of ensemble modelling have been acknowledged by the lake modelling community, until now no software to run multiple lake models for a single study site was available. LakeEnsemblR provides the necessary tools to widely apply ensembles of 1D lake models. Additionally to facilitating pre-processing of data, running of an ensemble of models, and standardising output, LakeEnsemblR allows the aquatic science community to start rigorous intra-model comparison studies of alternative process-based vertical 1D hydrodynamic lake models. Prior to the development of LakeEnsemblR, having an ensemble of models bound together with a consistent application programming interface, rigorous tests and comparison of alternative model codes were rare. We sincerely hope that LakeEnsemblR can provide a consistent framework for lake ensemble studies, uncertainty partitioning investigations, and intra-comparison modelling studies.

Author contributions

T.N.M., J.P.M., R.L., and J.F. conceptualised the study. T.N.M., J.P.M., R.L., and J.F. wrote most of the package code, with contributions of R.P., T.S., and J.R. T.N.M., J.P.M., R.L., J.F., F.O., R.P., J.J.V., and J.R. tested the package during development. T.N.M., J.P.M., R.L., and J.F. wrote the manuscript, with input from the other authors. All authors participated in discussions during package development and the publication process.

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Software and data availability

The LakeEnsemblR code is available at https://github.com/aemon-j/LakeEnsemblR. LakeEnsemblR and the packages it relies upon (FLakeR, GLM3r, GOTMr, SimstratR, MyLakeR, glmtools, gotmtools) can be installed in R following the instructions on the GitHub page, using the *install_github()* function of the devtools package (Wickham et al., 2020). The packages to run the models do not contain the source code of each model, only the executables for Windows, MacOS, and Linux. Links to the websites of the respective models are provided on GitHub. Example set-ups of LakeEnsemblR are provided at https://github.com/aemon-j/LER_examples. For further instructions on how to run LakeEnsemblR, we refer the reader to the AEMON-J GitHub page (https://github.com/aemon-j/LakeEnsemblR), where a vignette and a Wiki are available with detailed instructions and code examples.

LakeEnsemblR version 1.0.0 and the model packages have been archived in Zenodo under the following DOIs:

- LakeEnsemblR: 10.5281/zenodo.4146899
- FLakeR: 10.5281/zenodo.4139807
- GLM3r: 10.5281/zenodo.4146848
- GOTMr: 10.5281/zenodo.4139780
- SimstratR: 10.5281/zenodo.4139731
- MyLakeR: 10.5281/zenodo.4067998

When using LakeEnsemblR for a publication, please also cite the sources of the respective models that you are including in your ensemble (see *citation("LakeEnsemblR"))*.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.envsoft.2021.105101.

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