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OPINION PAPER

A community-based framework for aquatic ecosystem models

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Abstract Here, we communicate a point of departure in the development of aquatic ecosystem models, namely a new community-based framework, which supports an enhanced and transparent union between the collective expertise that exists in the communities of traditional ecologists and model developers. Through a literature survey, we document the growing importance of numerical aquatic ecosystem models while also noting the difficulties, up until now, of the aquatic scientific community to make significant advances in these models during the past two decades. Through a common forum for aquatic ecosystem modellers we aim to (i) advance collaboration within the aquatic ecosystem modelling community, (ii) enable increased use of models for research, policy and ecosystem-based management, (iii) facilitate a collective framework using common (standardised) code to ensure that model development is incremental, (iv) increase the transparency of model structure, assumptions and techniques, (v) achieve a greater

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understanding of aquatic ecosystem functioning, (vi) increase the reliability of predictions by aquatic ecosystem models, (vii) stimulate model inter-comparisons including differing model approaches, and (viii) avoid 're-inventing the wheel', thus accelerating improvements to aquatic ecosystem models. We intend to achieve this as a community that fosters interactions amongst ecologists and model developers. Further, we outline scientific topics recently articulated by the scientific community, which lend themselves well to being addressed by integrative modelling approaches and serve to motivate the progress and implementation of an open source model framework.

Keywords Ecological modelling · Open source · Model development

Introduction

Mathematical models are one of the principal instruments of modern science, and are increasingly being acknowledged for their role in scientific understanding and ecosystem management practices (Frigg & Hartmann, 2006; Schmolke et al., 2010). The development and application of numerical aquatic ecosystem models has been a rapidly growing field in aquatic sciences, in particular since the 1990s, with progression of computer technology, increasing needs for quantitative management of aquatic environments and a desire for more quantitative approaches in ecology (Rigler & Peters, 1995). The applicability of these aquatic ecosystem models spans across a wide range of time scales (Fig. 1) and spatial scales (ranging from zero-dimensional to three-dimensional), and their widespread use and increasing importance are evident from recent exponential increases in citations of these models in the scientific peer-reviewed literature (Fig. 2).

While a review by Jørgensen (1995) identified the need to make advances in the ecological representation (complexity) of ecosystems as the main challenge for aquatic ecosystem models during the 1990s, little progress has been made in this area during the past two decades, despite their increasing use. We argue that this languid progress is not caused by a lack of knowledge about ecosystem functioning, but rather the limited extent of open communication, inadequate collaboration and lack of suitable structure to support the aquatic scientific modelling community (see Mooij et al., 2010). This is evident from the Ecobas Register of Ecological Models (http://ecobas.org/www-server/index.html) which indicates that >100 aquatic models

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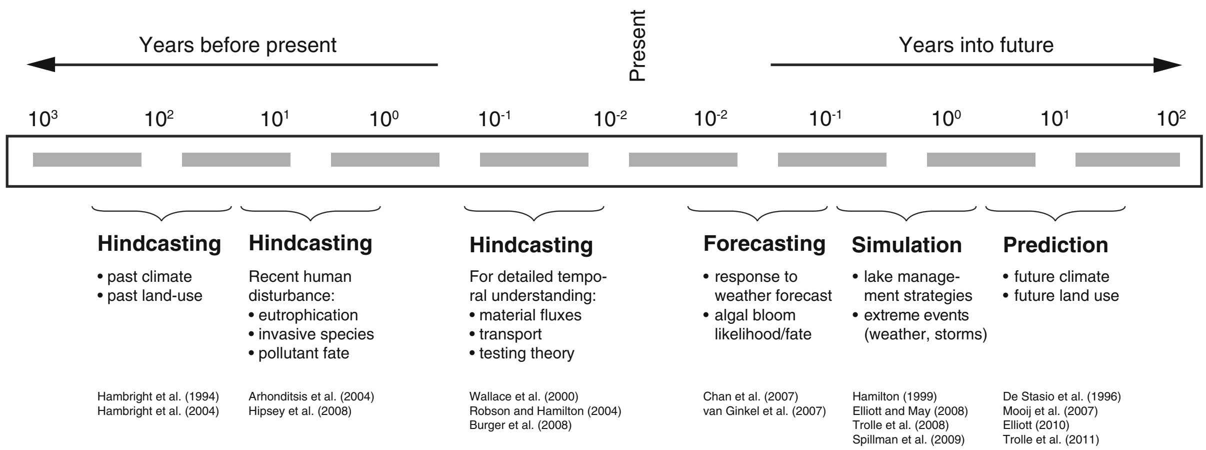
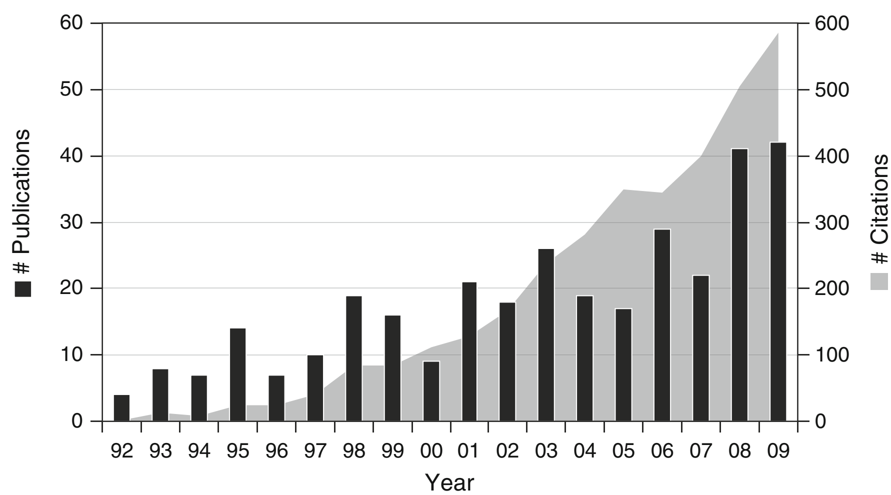


Fig. 1 Timescales, research topics and examples of associated peer-reviewed studies for applications of lake ecosystem models

Fig. 2 Publications and citations for each individual year based on ISI Web of Science database search on keywords "lake AND ecosystem AND model(l)ing", searching all citation databases (including years 1899–2009)



have been in existence in the past two decades, many of which have similar levels of ecological complexity and intent in terms of simulating selected components of aquatic ecosystems. This is in clear contrast to the progress made in climate modelling, where the scientific community has been able to focus and manage the development of a limited subset of well-respected climate models, and often apply these as an ensemble suite to quantify uncertainty of predictions (Pennell & Reichler, 2011). In the development of climate models, the Intergovernmental Panel on Climate Change (IPCC) has played a key role in moderating progress, managing the expectations around model certainty, stimulating model sensitivity analysis and across-scale (regional vs. global) validations, and acting as an interface between the modellers and the public (Randall et al., 2007).

We analysed literature relating to a subset of aquatic ecosystem models, including those described in Mooij et al. (2010), and those listed in the Ecobas Register of Ecological Models. Our literature search was limited to the medium "aquatic" and keywords "lake(s)" and to those with an acronym/name unique to the model (limiting the dataset to 18 different models). The results indicate that once developed many of the models are seldom if ever used and rarely cited in the peer-reviewed literature (Fig. 3). This analysis emphasizes the phenomenon identified by Mooij et al. (2010) of 're-inventing the wheel' whereby much of the lengthy phase of development of new models repeats all but a fraction of the content of existing models. Consequently, many of these models quickly become obsolete and generate negligible contribution to the wider modelling community and scientific knowledge. Only a few models, exemplified by a selection of four of the most cited models (Fig. 3), have demonstrated increasing use evident through a rise in publications and citations (Fig. 4) albeit that it has taken 5–10 years from the initial publication of the models before the initiation of a rapid increase in citations. However, these models either have restrictions on access to source codes, or limited flexibility and/or complexity in their hydrodynamic and/or ecological modules, thereby complicating further improvements.

Point of departure

In this article, we communicate a point of departure for the future development of aquatic ecosystem models. Twenty-five modellers from twelve different countries gathered together for a three-day workshop on Lake Ecosystem Modelling held in Silkeborg, Denmark in September 2010. This group initiated an open forum for aquatic ecosystem modellers—a new grassroots network. The objective of this network, now known as the Aquatic Ecosystem MOdelling Network (AEMON), is to promote and engage in development of open source models, released under the GNU General Public License (http://www.gnu.org/licenses/gpl.html), so that there is open sharing and exchange of common versions of models, and the models and model approaches being explored remain as open software for all users. This approach is not intended to solve the ambiguities scientists have in conceptualizing model structure, but rather through AEMON we aim to (i) advance collaboration within the aquatic ecosystem modelling community, (ii) enable increased use of models for research, policy and ecosystem-based management, (iii) facilitate a collective framework, using common (standardised) code, to ensure that model development is incremental, (iv) increase the transparency of model structure, assumptions and techniques, (v) achieve a greater understanding of aquatic ecosystem functioning, (vi) increase the reliability of predictions by aquatic ecosystem models, (vii) stimulate model inter-comparisons including

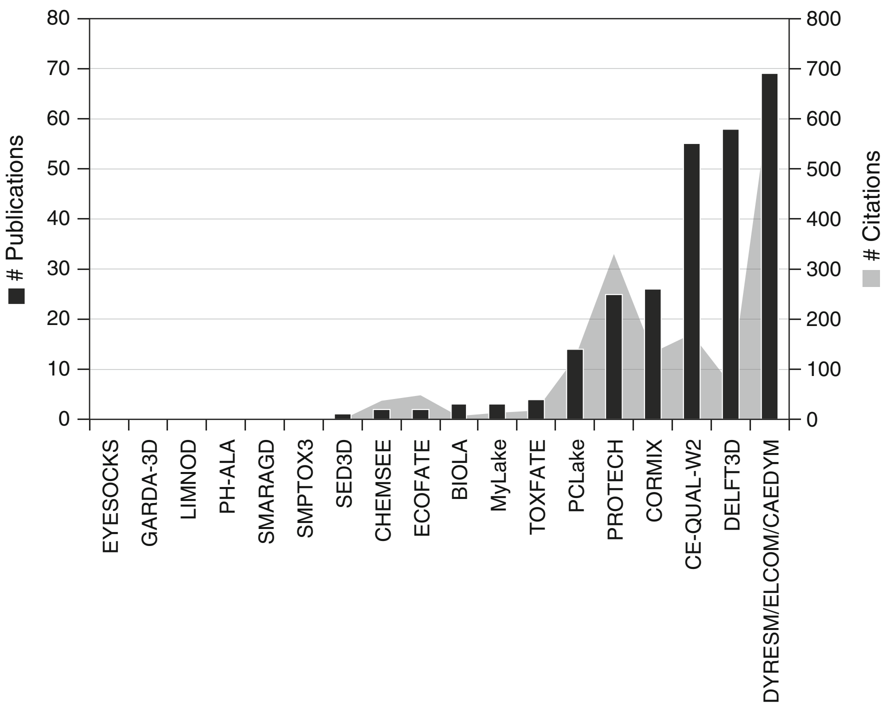


Fig. 3 Publications and citations for individual aquatic models listed in the Ecobas Register of Ecological Models (REM, http://ecobas.org/www-server/index.html). Number of publications and citations were based on ISI Web of Science database search using the model acronyms as keywords. Models included from REM were limited to the medium "aquatic" and keywords "lake(s)" and further limited to those with an acronym/name unique to the model (e.g., the model "foodweb" was excluded from the citation analysis). Three additional models were added based on a recent modelling review by Mooij et al. (2010)

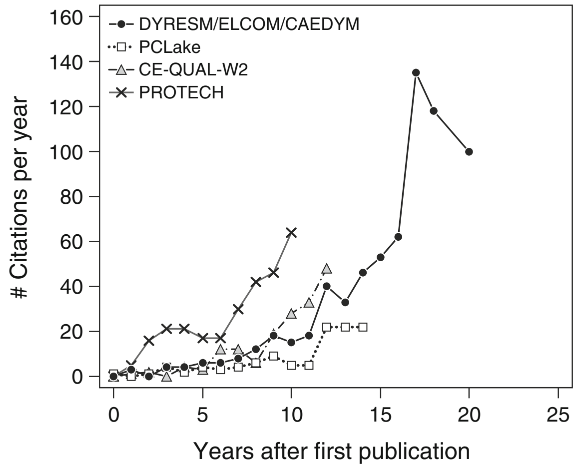


Fig. 4 Scientific citations of the lake ecosystem models DYRESM(1D)/ELCOM(3D)/CAEDYM (first publication in 1991), PCLake (first publication in 1995), CE-QUAL-W2 (first publication in 1997) and PROTECH (first publication in 1999). Citation data were based on ISI Web of Science database search using the model acronyms as keywords (self-citations are included)

differing model approaches, and (viii) avoid 're-inventing the wheel', thus accelerating improvements to aquatic ecosystem models.

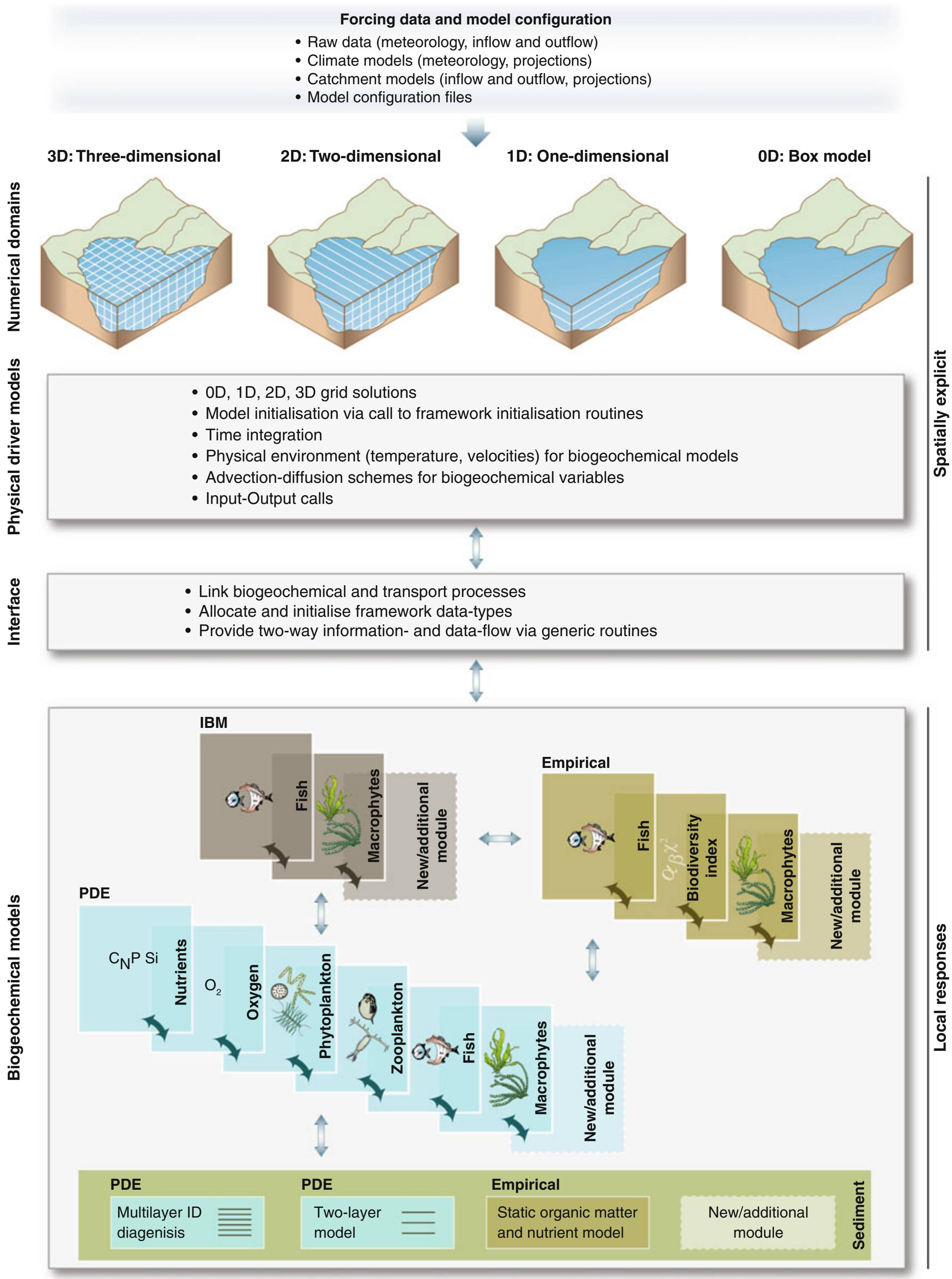
A community-based framework for aquatic ecosystem models

While it may take several years after a model has been developed by an individual modelling group before it is widely accepted and cited in the literature (exemplified by the 5–10-year lag-phase in citations in Fig. 4), there are ways to greatly increase the exposure of new model developments as a community. Through use of a common vocabulary and standards, agreed scientific hypotheses, and experiments with model structures, different model approaches can be better explored and scrutinized. It is envisaged that this approach will facilitate inter-disciplinary research by ensuring specializations common to individual researchers can be linked together within an inter-disciplinary scientific network that is predicated upon a community-based modelling framework.

Our overall goal is to develop a new community-based framework for aquatic ecosystem models which is flexible and readily expandable to allow model users and developers to couple a diverse array of hydrodynamic or hydrological drivers to one or several types of biogeochemical and/or ecological modules (Fig. 5). Hence, it is not our intention to develop a one-for-all "super model", but rather a framework that readily allows the use of a range of different models—of various complexities—which can be used and further adapted, based on the purpose and data availability of a given modelling exercise. By decoupling the requirement that a particular ecological model is tied to specific physical transport models we will be able to more efficiently apply the model across a diverse range of aquatic environments (e.g., wetlands, lakes, rivers and coastal waters) and support our search for commonalities between systems and, through synthesis activities, define universal descriptors of processes. The challenge is to develop a generic and flexible interface approach where biogeochemical and ecological processes are 'split' from the components dealing with transport and mixing. While such an approach has been demonstrated widely with individual physical models and physical processes, such a system has so far not been employed within the aquatic sciences community for coupling of biogeochemical and ecological modules to a diverse array of physical model approaches and grid types. In practice such a flexible system may only be realized through community-based development capitalizing on collaboration amongst modellers, ecologists, and physical limnologists who invest in the substantial setup and validation efforts at individual sites. An example of such a framework is the Fortran-based Framework for Aquatic Biogeochemical Models (FABM, http://sourceforge.net/projects/fabm/, developed as part of the European FP7 project Marine Ecosystem Evolution in a Changing Environment). Experiences from the early development of this framework have identified two cornerstones that are essential for a generic framework to succeed.

Cornerstone 1: localized interaction in time and space

To achieve independence of the specifics of hydrodynamic and hydrological drivers, biogeochemical and ecological modules cannot make assumptions of the dimensionality and structure of their (modelled) environment. By default, this suggests that the underlying processes are best modelled as local responses at a single point in space and time: based on the *local* value of environmental and biogeochemical variables,


Forcing data and model configuration
• Raw data (meteorology, inflow and outflow)
• Climate models (meteorology, projections)
• Catchment models (inflow and outflow, projections)
• Model configuration files
3D: Three-dimensional
2D: Two-dimensional
1D: One-dimensional
0D: Box model
Numerical domains
Physical driver models
• 0D, 1D, 2D, 3D grid solutions
• Model initialisation via call to framework initialisation routines
• Time integration
• Physical environment (temperature, velocities) for biogeochemical models
• Advection-diffusion schemes for biogeochemical variables
• Input-Output calls
Interface
• Link biogeochemical and transport processes
• Allocate and initialise framework data-types
• Provide two-way information- and data-flow via generic routines
Spatially explicit
Biogeochemical models
IBM
Fish
Macrophytes
New/additional module
Empirical
Fish
Biodiversity index
Macrophytes
New/additional module
PDE
CNP Si
Nutrients
O2
Oxygen
Phytoplankton
Zooplankton
Fish
Macrophytes
New/additional module
Local responses
PDE
Multilayer ID diagenisis
PDE
Two-layer model
Empirical
Static organic matter and nutrient model
New/additional module
Sediment

◀ **Fig. 5** A framework for a flexible modelling system for aquatic ecosystem models, including a range of hydrodynamic drivers and ecological/biogeochemical modules/packages, which can be developed and modified by the scientific community. Examples of ecological packages would be PDE (mass balance-based partial differential equation), IBMs (Individual Based Models) and empirical models

such modules modify the system by providing *local* sink and source terms. The responsibility for the final integration of these local terms across the full spatial domain and in time comes to lie with the physical driver, which generally includes the logic (e.g., numerical schemes for advection, diffusion, time integration) for this specific purpose. By casting biogeochemistry and ecology as local processes, the way is open for closer integration of Eulerian (population/community) and Lagrangian (individual-based, IBM) models, similar to the approaches recently demonstrated by Makler-Pick et al. (2011). A modelling framework built upon local responses to local conditions should just as easily couple a population model to a grid-based physical driver, as is the case for an IBM to a Lagrangian transport model. Ultimately, we envisage that such a framework will allow for the application of hybrid models (i.e., mixed modelling approaches), which have defined sets of variables packed together in particles or individuals, and responding to local conditions. Hence, the framework could contribute to the bridging of the traditionally distinct worlds of population modelling and IBMs (Grimm et al., 2005).

Cornerstone 2: module isolation with supervised information sharing

No model of a specific biogeochemical or ecological process is an island. Their response nearly always depends on the physical environment (e.g., temperature, light). In addition, the response will often depend on biogeochemical variables outside their specific model domain. For instance, a model of phytoplankton will depend on nutrient availability, which may be described by a specific, detailed model for the inorganic nutrient cycle. Ideally, models would be coded once, by scientists closest to the subject matter, and then shared. The resulting modules should integrate dynamically (i.e., at run time, not compile time) in coupled models of food webs and elemental cycles. This requires that individual modules are self-contained and agnostic about each other's presence. To achieve this, modules should register both the variables they describe and the external environmental and biogeochemical variables they depend on, but they must relinquish control over the location of the variable values. A modelling framework should therefore include pre-processing macros that handles these operations, and should maintain up-to-date values for all variables, and pass these to individual modules when needed. Through this division, a coupling/communication layer (part of the framework) can be nested between the central variable store and individual modules, allowing it to link variables from the different biogeochemical and ecological modules (as well as those residing in the physical driver) according to user-supplied, simulation-specific settings. Such a construction permits dynamic recombination of biogeochemical modules in large coupled models. Moreover, it places this functionality in the hands of users, not programmers. An early demonstration of the feasibility of such a generic framework is found in the Framework for Aquatic Biogeochemical Models (FABM), which, while in an early stage of development, is already capable of hosting multiple coupled biogeochemical modules and connecting to several 1D and 3D hydrodynamic drivers. On top of FABM, a highly generic, modular aquatic ecosystem model is currently being developed (M. R. Hipsey, unpublished), which is based on the philosophy of the two cornerstones outlined in this article. This consists of a collection of flexible model objects implemented in Fortran 2003, this language is chosen to maximise compatibility with existing codes and hydrodynamic drivers. Each model object will focus on a key ecosystem component (e.g., nutrients, phytoplankton, organic matter, macrophytes, fish), and constructed so users can easily add/remove variables within a model component with limited coding (e.g., multiple phytoplankton groups in the phytoplankton module), or alternatively port in existing code. The framework is also designed to embrace mixed-modelling approaches and thereby facilitate linking of modules that adopt different underlying model approaches. Cross-module dependencies (e.g., phytoplankton module depends on nutrient module) are able to be setup by registering them within a central coupling layer, as proposed above. Importantly, through its description of spatially localized interactions and abstraction from the physical driver, the code library allows coupling with a diverse range of hydrodynamic model grids, thereby encouraging adoption of the model across a range of environmental applications.

Scientific topics addressed by the community

The motivation for engaging in open source model development, which will also benefit others who may apply the models, will primarily be to advance scientific understanding using the models as a tool to predict and potentially to manage ecosystem behaviour. During the AEMON workshop in Silkeborg, a list of eight currently pertinent scientific topics was outlined, which lend themselves well to being addressed by the community. These topics include:

- application of the ensemble suite of model conceptualizations developed through AEMON to elucidate the influence of model complexity on predictive capability;
- exchanging data from a globally distributed network of lake observatories for a generalized model validation across broad ranges of time scales and key ecosystem gradients, such as lake size, mixing regime, trophic status, and geological and land-use settings;
- development of models that include state variables which directly or indirectly can be used as indicators and predictors of biodiversity and functional diversity;
- coupling of aquatic ecosystem models with meteorological models and catchment models to quantify responses of aquatic ecosystems (structure and process rates) to climate change and land use change across the globe;
- development and application of models that include sufficient complexity to reflect multiple responses of aquatic ecosystems to perturbations and anthropogenic forcings, including resilience, hysteresis and non-linearity;
- development of aquatic ecosystem models that equally well encompass top-down (predation and grazing dependence) and bottom-up (microbial loop and nutrient dynamics) effects for application in ecosystem based management, including fisheries;
- elucidating and untangling pathways of elemental cycles and stoichiometric transitions through improvements in model conceptualization and representation of food webs, the microbial loop and sediment–water interactions;
- standardising calibration and uncertainty estimation techniques, and elucidating the uncertainty underlying model structures and parameters, thereby enabling the ability to obtain weighted averages of the predictions as well as uncertainty, from different models developed for the same system.

Summary and conclusions

In this article, we communicate a point of departure in the development of aquatic ecosystem models, namely a new community-based framework, which supports an enhanced and transparent union between the collective expertise that exists in the communities of traditional ecologists and model developers. An initial basis of the framework, derived from open collaboration within the community, has already been documented in the review paper by Mooij et al. (2010), which sets the scene for the open aquatic modelling community through a review of the existing lake ecosystem models and identification of the main pitfalls that the development of these models exhibits. A public website has also been set up, with the main purpose of sharing information, ensuring ongoing open communication, and to provide a discussion forum (https://sites.google.com/site/aquaticmodelling/). It is our intention to ensure that progress is made on the model framework through additional workshops—to be announced on the public website—thus motivating development and application of models within the framework and providing ongoing support to the community. Other grassroots organisations such as the Global Lake Ecological Observatory Network (GLEON) have specific aligned working groups (e.g., Ecosystem Modelling) that offer an additional opportunity to more rapidly advance the community-based modelling framework through common researchers, provision of high-frequency data suitable for rigorously testing models, and disseminating the use of the models in a broader ecological community. These types of activities will also help to identify and resolve the impediments to an open source model framework that is essential for addressing the current scientific and management challenges for aquatic systems across the globe.

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