Dear Editor, referees and other interested members:

On behalf of the authors for the model description paper entitled "FABM-PCLake: linking aquatic ecology with hydrodynamics", we thank referees for dedicated and insightful comments. Please find our specific point-by-point responses to the referees' comments below. The original comments by the referees' are noted in *Italics* and our replies are provided in standard font.

As part of the peer-review process, we have also improved the model code structure. This entailed further modularization of the code, which ultimately makes the model more user-friendly and also provides greater flexibility to adapt the conceptual model to individual systems. The code has been updated in the public repository. The code changes have not affected the biogeochemical processes of FABM-PCLake described here, but simply the way they are divided into different modules in the code. Please see the specific details provided under 'Additional revisions' at the end of this letter.

Yours sincerely,

Fenjuan Hu

Reply to referee Nr.1

General Comments:

This manuscript is a concise description of the connection of PClake to FABM. This is a very powerful advancement and certainly of interest for the readership of GMD. The PClake-model is an ecological model of shallow lakes frequently used in science and management. Since shallow lakes are classically viewed as stratified (i. e. mixed) systems, PClake is originally a 0D model, i.e. it models the lake as one mixed box. By connecting this model, which contained a high and reliable amount of ecological processes, to FABM it can also be applied outside the 0D context and coupled with physical models for 1D or 3D hydrodynamics. This is a real step forward and certainly deserves publication. The MS is well written and well understandable. I have not seen major flaws or mistakes but I think that the scientific content of the paper could be improved. In its current form, the MS reads more like a newsgroup contribution and not yet like a full research paper. This would be different if 1-2 more applications would be shown. I also have a few questions about the details/consequences of the coupling and a few very minor points (see below).

I want to point out that *I* highly valued the excellent supplement material of this paper, which provides the experienced modeller with very helpful knowledge and facts.

Reply: Thank you for the comprehensive summary of our work and the positive feedback relating to the supplementary material. In terms of the form (i.e. style) of the paper, we have followed the guidelines of GMD's "Model description papers". This include aspects relating to the scientific basis and purpose, the technical details of the model implementation (i.e. overview the numerical solution and the modular structure design), model verification (benchmark test), main model features as well as perspectives in relation to applications and further developments. We have included a new model application example, as suggested, which demonstrate a one year simulation of temperature and macrophyte profiles as

simulated by FABM-PCLake coupled with the one-dimensional physical model GOTM, which include a hypsographic representation of the sediment-water interface (Fig.5). This plot also relates to the reviewers' comments' #1, #2 and #3, which we comment further on below.

Major comments:

1. The paper would be improved if the abilities of the model would be shown with 1-2 more applications. This could be a simplified setting of a 3D model or a comparison of a 0D and a 1D simulation for a given system or a comparison of observed and modeled 1D dynamics in a given lake.... It would just leave a clearer impression of the abilities of the model system, particularly to those readers that have not yet heard from FABM et al

Reply: As an additional example and manifestation of the models abilities, we have now included a new model application example, as suggested, which demonstrate a one year simulation of temperature and macrophyte profiles as simulated by FABM-PCLake coupled with the one-dimensional physical model GOTM. Output from the model application example is demonstrated in the new Fig. 5. We also provide details relating to the concept of the sediment-water interface of this 1D application, which also relate to comment #2 and #3 below.

2. In the classical shallow lakes paradigm one has either a state with the dominance of pelagic primary producers (algae) or a state with the dominance of benthic primary producers (macrophytes). As soon as you move the PClake-model in a 1D-setting, every depth layer gets an own sediment surface attributed to this layer (derived from the bathymetric map). I expect that this spatial representation affects the competition between benthic and pelagic primary producers – the shallower a given 1D layer is located within the water column, the more superior becomes the benthic primary producer (because it gets more light). It is not clear to me, how exactly the benthic and pelagic compartments interact in a 1D setting – does each layer indeed have two separate ecological compartments (pelagic vs benthic?)? In the original 0D-setting everything is simple and clear because the benthic compartment is on the lake bottom and the pelagic compartment on top of this. In the 1D setting, benthic and pelagic compartments coexist side by side within the same layer? Does that mean that the algae can never fully exclude macrophytes from the lake because the macrophytes can persist in the benthic compartments of the shallow layers (which may be a realistic condition?)??? Anyway – please explain in more detail. And keep in mind that this may become even more complex in a 3D-setting.

Reply: FABM-PCLake will function with any of the physical models for which a FABM interface has been written. This currently includes 0D, 1D as well as 3D models. The benthic-pelagic coupling is defined by the design of this interface. In practice, this means that as a model user, one can choose which physical representation is most suitable for the application purpose. For example, one can run FABM-PCLake with a standard GOTM (1D) set up, which means that only the most bottom layer will have a sediment-water interface. Alternatively, one can run FABM-PCLake with GOTM (1D) using a hypsographic representation of the sediment-water interface (simply by "turning ON" a hypsograph feature in GOTM), meaning that each individual water column layer is coupled to a certain sediment area (the size of this area relates to the hypsograph of the lake, which must then be provided as an input by the user). A

model user may also choose a 3D model (e.g. GETM), which will then represent sediment-water interfaces for the bottommost cells in a three-dimensional domain. Hence, benthic and pelagic compartments can interact in both 1D and 3D settings, and in practice you would see that macrophytes may be present in the uppermost layers in a 1D model (with hypsograph), while being absent from deeper layers. To demonstrate this point, we have included an additional model application example (Fig. 5), where FABM-PCLake is coupled to GOTM using a hypsographic representation. Here, macrophytes are present in the uppermost layers (in this example extending to 4-5 meters depth), while at the same time being absent from deeper layers (where, for example, light conditions may not suffice for growth). The depth extent for macrophytes is influenced by light availability, temperature and nutrient concentrations in the sediments. Hence, macrophytes and phytoplankton in FABM-PCLake will compete for light, and if phytoplankton concentration increases, the depth extent of macrophytes will decrease (or potentially be absent altogether). We think this is a more reliable description than the classical on-off (regime shift assumption) for shallow lakes. While on-off (clear-turbid) may be true for lakes that have a very flat bottom, most lakes have variable depth and show more gradual response to changes in loading such as the Danish lakes (see Jeppesen et al., 2007, for example).

3. In a real lake, macrophytes grow into the pelagic compartment and can even fully occupy the pelagic compartment. Is it in the 1D setting allowed, that macrophytes can grow from there (home-) benthic upward into the next (pelagic) one above?

Reply: Yes, the macrophytes in this case can extend into pelagic layer based on its height, and thereby influence light attenuation. The macrophyte code is at present similar to the original PCLake, meaning that the macrophyte height is specified simply by the user. In terms of perspectives relating to further code developments, it would be interesting to enable a dynamic macrophyte height simulation, e.g. similar to what has been presented by Sachse et al. (2014).

Reply to referee Nr.2:

This paper announces through a brief communication the coupling of PCLake to a variety of hydrodynamic models of various spatial representations (0D, 1D, 3D) via the Framework for Aquatic Biogeochemical Models (FABM). Of particular significance is (1) fully coupled linkage and feedback between PCLake and the physical model, (2) open source code with supporting contact persons, (3) compilation of code using Public License software, and (4) tailored output modules for comprehensive visualization.

The abstract states that the study involves a complete redesign of the PCLake model, but I would argue this is not the case and that the changes to the internal structure of of PCLake are largely incremental (e.g., sediment resuspension representation). The link to the hydrodynamic models is, however, a "redesign". I regard announcement of the new PCLake-FABM code as important and the paper fits within the scope of material of interest to the readers of GMDD. My only other major comments are that it would be useful to have references associated with the new model developments (p. 5) including sediment resuspension and the additional options to describe light limitation of phytoplankton.

Reply: We have now changed the wording in the abstract to: "This study presents FABM-PCLake, a redesigned structure of the PCLake aquatic ecosystem model, which...".

We have added additional references relating specifically to the background of the new features that we developed in relation to resuspension methods and light functions .

Minor comments:

1) The abstract has repetition; the physical models for heteroge- neous environments (l. 7, l. 17).

Reply: we have now changed the wording to avoid repetition on lines 7 band 17, respectively.

2) The term "worldwide" at the bottom of the abstract is very open. A better specification would be useful.

Reply: We have revised the text from "for lakes and reservoirs wordwide" to "for temperate, subtropical and tropical lakes and reservoirs".

3) Coupled 1D models of physics and water quality have been around for 2-3 decades – the text on p. 3, l. 4 could be more specific that few, if any, coupled models are actively used which have detailed representations of higher trophic level processes.

Reply: We have revised this sentence as followed, now including additional references:

"Few studies have attempted to couple aquatic ecosystem dynamics (e.g., Hamilton and Schladow, 1997; Pereira et al., 2006; Fragoso et al., 2009), sometimes also including higher trophic levels (Makler-Pick et al., 2011). However, none of these models are validated for higher trophic levels (i.e., fish) or readily available for further development."

4) p. 4, l. 12: these physical pro- cesses are a subset of mixing and diffusion .

Reply: The reviewer is correct, and we have now clarified this sentence (eddy-mixing is no longer mentioned explicitly).

5) p. 4, ll. 14-23: the text here was confusing and requires revision.

Reply: We have now tried to clarify the text in this particular section, which also refers to Bruggeman and Bolding 2014 for full details. The section now reads:

"Therefore, based on local variables (including, for example, local light conditions, temperature and concentrations of state variables) provided by a hydrodynamic model, the biogeochemical model calculate rates of sink and source terms at current time and space and pass the rates to the hydrodynamic model via FABM. The hydrodynamic model will then handle numerical integration of the biogeochemical processes and transport, and then pass updated states via FABM back to the biogeochemical model – and this process will continue until the user-defined end-time of a simulation."

6) p. 4, ll. 30-31: please associate references with the model.

Reply: We have added references for the specific models mentioned and updated the reference list accordingly.

7) p. 5, l. 3: FABM-PCLake can now be linked to physical process models.

Reply: Text has been changed accordingly.

8) p. 5: what is actually passed between the models; a shear stress from the physical model that enables material to be moved from bottom sediments to water? Fig. 1: indication rather than illustration? Could this diagram have something that really looked like a real fish?

Reply: Bottom shear stress is calculated by a physical model and then passed through FABM to the biogeochemical model. We have replaced the word "illustration" with "indication" in the caption for Fig.1. We have revised this part with more caution in specifying these points, now reads as followed:

"For example, while the resuspension rate of detritus (represented by an arrow going from the bottom sediments to the water column in Fig. 1) is derived from an empirical relation to lake fetch in the original PCLake, resuspension rate in FABM-PCLake can now be derived from the actual bottom shear stress as computed by the physical model and passed via FABM to the biogeochemical model."

Fig. 2: I assume that phytoplankton are not restricted to these three groups?

Reply: The original PCLake model comprises three groups of phytoplankton (as depicted in the figure). This is also the standard configuration of FABM-PCLake. However, FABM allows coupling of individual biogeochemical models at runtime. Hence, a model user may simply configure a simulation to include none, one, two, three (etc.) FABM-PCLake-phytoplankton modules. Thereby, the user has control of the complexity of the conceptual model and, for example, how many phytoplankton groups to include (and can also parameterize each phytoplankton group individually through input files, without the need to revise code).

p. 5, l. 29: bases p. 5, l. 30: this description appears to imply that PAR in a cell is not depth integrated; the use of a centre point is not technically correct because of the exponential attenuation of light with depth.

Reply: The text refers to how cell centre point PAR is passed between physical models and biogeochemical models – and not how these values are processed by light functions to derive primary production. There are multiple light functions implemented in biogeochcemical models in FABM; some utilize centre point PAR while others use the PAR value at top and bottom of a layer for deriving depth integrated PAR.

What is meant by the following: p. 6, l. 16: "enforce certain components" p. 6, l. 21: "overall system processes" p. 6, l. 23: "can prevent a net increase of sediment material". The latter relates to the fact that sediment accumulates naturally in all lakes, so some clarification is required.

Reply: We have revised this part, which now reads:

"The overall system processes are the processes that typically influence several other modules, and they include resuspension, sedimentation and burial. In PCLake, burial is included as a representation of the natural process of sediment accumulation, which is caused by excessive sedimentation (resuspension rate < sedimentation rate) of particles at the sediment-water interface. The "buried" material is then considered inactive in the sediment biogeochemical processes and excluded from the system. "

The comparison of the "old" and "new" PCLake results (Fig. 3) is impressive but I do not understand how they were almost identical with different resuspension Models? Wouldn't it had been easier to have switched off resuspension or was there calibration involved or did resuspension simply not occur?

Reply: This is a benchmark test, for which the main purpose is to test that the new model can produce identical output relative to the old model. Therefore, and as specified on p. 7, both the 'old' and 'new' PCLake model simulation make use of the same (old) empirical resuspension function for this comparison.

p. 7, l. 30: spatially p. 8, l. 8: "look at" = "simulate"

Reply: We have changed text accordingly.

Additional revisions since original submission:

Revision of FABM-PCLake code and module structure

To be completely consistent with the modular design philosophy of FABM, the FABM-PCLake's original foodweb_water module have been separated into a zooplankton and fish module, respectively. Accordingly, foodweb_sediment module has been renamed as zoobenthos. This separation enables greater flexibility when designing the conceptual model for a specific system as modules may be turned On or Off, repeated several times (e.g. to include multiple zooplankton groups rather than just a single group) or replaced by another biogeochemical module available within FABM. The names of the modules and source files have been changed accordingly. The source files, the Supplementary Material and Fig. 2 have been updated accordingly.

References:

Jeppesen, E., M. Søndergaard, M. Meerhoff, T.L. Lauridsen & J.P. Jensen, 2007. Shallow lake restoration by nutrient loading reduction – some recent findings and challenges ahead. Hydrobiologia, 584,239-252.

Sachse, R., Petzoldt, T., Blumstock, M., Moreira, S., Pätzig, M., Rücker, J., Janse, J.H., Mooij, W.M. and Hilt, S., 2014. Extending one-dimensional models for deep lakes to simulate the impact of submerged macrophytes on water quality. Environmental Modelling & Software, 61, 410-423.

1 FABM-PCLake – linking aquatic ecology with

2 hydrodynamics

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1 Abstract

2 This study presents FABM-PCLake, a complete redesigned structure of the PCLake 3 aquatic ecosystem model, which we implemented into the Framework for Aquatic 4 Biogeochemical Models (FABM). In contrast to the original model, which was 5 designed for temperate, fully mixed freshwater lakes, the new FABM-PCLake 6 represents an integrated aquatic ecosystem model that can be linked with different 7 hydrodynamic models and allows enables simulations of hydrodynamics and biogeochemical processes for zero-dimensional, one-dimensional as well as three-8 9 dimensional heterogeneous environments. FABM-PCLake describes interactions 10 between multiple trophic levels, including piscivorous, zooplanktivorous and 11 benthivorous fish, zooplankton, zoobenthos, three groups of phytoplankton and 12 rooted macrophytes. The model also accounts for oxygen dynamics and nutrient 13 cycling for nitrogen, phosphorus and silicon, both within the pelagic and benthic 14 FABM-PCLake includes a two-way communication between the domains. 15 biogeochemical processes and the physics, where some biogeochemical state variables (e.g., phytoplankton) influence light attenuation and thereby the spatial and 16 17 temporal distributions of light and heat. At the same time, the physical environment, including water currents, light and temperature influence a wide range of 18 19 biogeochemical processes. The model enables studies on ecosystem dynamics in physically heterogeneous environments (e.g., stratifying water bodies, and water 20 21 bodies with horizontal gradient in physical and biogeochemical properties), and 22 through FABM also enables data assimilation and multi-model ensemble simulations. 23 Examples of relevant potential new model applications include climate change impact 24 studies and environmental impact assessment scenarios for temperate, sub-tropical 25 and tropical lakes and reservoirs worldwide.

26

27 **1** Introduction

The field of aquatic ecosystem modelling has undergone waves of development during the past decades, and models have grown in complexity in terms of ecosystem components and processes included (Robson, 2014). However, even though hundreds of models have been formulated for research or management purposes, only a handful has found frequent use and ongoing development (Trolle et

1 al., 2012). This reflects that many models are being built with the same or similar 2 properties, and thus that model development for the past decades has been subject 3 to some degree of "re-inventing the wheel" as discussed by Mooij et al (2010). 4 Another drawback of many aquatic ecosystem models is the typical discrepancy in 5 complexity between the ecosystem representation and the physical environment. 6 Hence, few studies have attempted to couple aquatic ecosystem dynamics including 7 higher trophic levels (e.g., fish) and explicit physical dynamics (one example is the 8 study by Makler-Pick et al. (2011)), which, however, is not readily available for further 9 developments). High complexity in ecosystem conceptualizations therefore generally 10 comes at the expense of simple or no hydrodynamic representation (e.g., PCLake 11 (Janse and van Liere, 1995; Janse, 2005; Janse et al., 2008) and EcoPath 12 (Christensen and Pauly, 1992)). By contrast, physically resolved hydrodynamic 13 models often include no or only simple ecosystem representations, and disregard 14 higher trophic levels. <u>Few studies have attempted to couple aquatic ecosystem</u> 15 dvnamics (e.g., Hamilton and Schladow, 1997; Pereira et al., 2006; Fragoso et al., 16 2009), sometimes also including higher trophic levels (Makler-Pick et al., 2011). 17 However, none of these models are validated for higher trophic levels (i.e. fish) and 18 the source codes are also not readily available for further development. To avoid "re-19 inventing the wheel", and to overcome this discrepancy in complexity between the 20 ecological and physical representation, a way forward is to enable an easy coupling 21 between existing ecosystem models and hydrodynamic models. Thus, the complexity 22 of the conceptual biogeochemical model and the physical representation may readily 23 be adapted to best suit the needs and purposes of a given study. Meanwhile, utilizing 24 an open source platform would help promote model availability and also further development (Trolle et al., 2012). To this end, we implemented and modified a well-25 26 developed and widely applied ecosystem model, PCLake, within FABM, the 27 Framework for Aquatic Biogeochemical Models by Bruggeman and Bolding (2014). 28 FABM enables a flexible coupling of ecosystem processes in PCLake with a 29 selection of hydrodynamic models representing zero- to three-dimensional 30 hydrodynamics.

2 Implementation of PCLake in FABM

2 PCLake is originally a zero-dimensional ecological model for shallow lakes 3 developed by Janse and van Liere (1995) and it has been widely applied (for 4 example, Stonevičius and Taminskas, 2007; Mooij et al., 2009; Nielsen et al., 2014; further references in Mooij et al., 2010). The model describes the dynamics of 5 6 phytoplankton, macrophytes and a simplified food web including zooplankton, 7 zoobenthos, zooplanktivorous fish, benthivorous fish and piscivorous fish, and 8 accounts for mass balances, represented by dry weight, nitrogen, phosphorus and silicon cycling between the various components of the ecosystem. The original 9 10 PCLake model (documented in detail in Janse (2005)) contains detailed biological processes within the water column and also a relatively advanced biogeochemical 11 12 sediment module (describing nutrient dynamics in the sediment top layer and exchanges with the water column), while thermo- and hydrodynamics are not 13 14 explicitly accounted for. The original model also includes a marsh module describing (helophytic) marsh vegetation in a zone around a lake, which attempts to account for 15 16 interactions between open waters and a more highly vegetated marsh area that may be present close to the shoreline of some lakes. The main purpose of the model is to 17 predict critical nutrient loadings, i.e. the loading where a shallow lake may switch 18 between a clear and a turbid state, related to a non-linear ecosystem response to 19 20 nutrient loading as a result of self-enhancing feedback mechanisms within the 21 ecosystem.

22 FABM, in which we have now implemented PCLake, is a framework for 23 biogeochemical models of marine and freshwater systems (Bruggeman and Bolding, 24 2014). FABM enables complex biogeochemical models to be developed as sets of 25 stand-alone, process-specific modules. These can be combined at runtime to create 26 custom-tailored models. As outlined in detail by Bruggeman and Bolding (2014), 27 FABM divides the coupled advection-diffusion-reaction equation that governs the 28 dynamics of biogeochemical variables into two parts: a reaction part (i.e., sink and 29 source terms) provided by the biogeochemical models, and a transport part handled 30 by the hydrodynamic (i.e., physical) models. The transport part includes advection, 31 diffusion and potential vertical movements (sinking, floating and potentially active 32 movement), and also dilution and concentration processes. Therefore, based on local

1 (including, for example, local light conditions, temperature variables and 2 concentrations of state variables) provided by a hydrodynamic model, the 3 biogeochemical model calculate rates of sink and source terms at current time and 4 space and pass the rates to the hydrodynamic model via FABM. The hydrodynamic model will then handle numerical integration of the biogeochemical processes and 5 transport, and then pass updated states via FABM back to the biogeochemical model 6 7 - and this process will continue until the user-defined end-time of a simulation. FABM 8 thereby enables model applications of different physical representations (ranging 0D 9 to 3D) without the need to change the biogeochemical source code. Most of the 10 pelagic state variables in a biogeochemical model implemented in FABM will typically 11 be transported by the hydrodynamics. However, some pelagic variables, particularly 12 relevant for higher trophic levels such as fish (that may exhibit active movement 13 based, for example, on the food source availability), can be set as exempt from 14 hydrodynamic transport or even include their own custom time and space varying 15 movement. On the other hand, all benthic state variables, such as macrophytes (that 16 need to be attached to a "benthic" grid cell), are always exempt from hydrodynamic 17 transport. Further detail on the concept of FABM is provided in Bruggeman and 18 Bolding (2014).

19 Besides PCLake, a series of large ecosystem models haves been implemented in 20 FABM. These include representations of the European Regional Seas Ecosystem 21 Model (ERSEM, Butenschön et al., 2016) and the lake model Aquatic EcoDynamics 22 (AED, <u>Hipsey et al., 2013</u>). But in contrast to PCLake, none of these include higher 23 trophic levels such as fish. FABM is written in Fortran2003 and therefore FABM-24 PCLake is also implemented in Fortran2003. The key difference between the new 25 FABM-PCLake (Fig. 1) and the original PCLake conceptual model (e.g., Janse et al. 26 2010) is that FABM-PCLake can now be linked toenables physical modelss. Hence, 27 a major advantage of FABM-PCLake is that the detailed biogeochemical processes 28 provided by PCLake can now be used to study deep (i.e. stratifying) and spatially 29 complex aquatic ecosystems. While the core of the overall conceptual model of the 30 PCLake "lake part" remains intact, the underlying mechanisms of processes that 31 relate to transport have changed. For example, while the resuspension rate of 32 detritus (represented by an arrow going from the bottom sediments to the water 33 column in Fig. 1) is derived from an empirical relation to lake fetch in the original 1 PCLake (represented by an arrow going from the bottom sediments to the water 2 column in Fig. 1), resuspension rate in FABM-PCLake can now be derived from the 3 actual bottom shear stress as computed by the physical model simulated by and 4 passed via FABM to the biogeochemical model. When implementing PCLake into 5 FABM, a series of modifications relative to the original PCLake model were made. This was done because some of the processes parameterized in the original PCLake 6 7 model can now be resolved explicitly by the hydrodynamic models and the 8 functionalities of FABM.

9 The main modifications are:

- excluding the marsh module (as any two- or three-dimensional exchanges of
 solutes can now be resolved by an explicit physical domain);
- 2) excluding the original loading, dilution and water level burial correction
 processes (as this will now instead be resolved by the physical model and its
 boundary conditions);
- 3) excluding the original (and optional) forcing for dredging processes and fish
 harvesting (as similar functionality is now provided through the state variable
 time series forcing enabled by FABM);
- 4) adding the option to make resuspension directly dependent on bottom shear
 stress provided by the hydrodynamic model. This functionality is derived from
 the PCLake integral resuspension function and the shear-stress correlated
 resuspension function by Hamilton (1996) and may now be used as an
 alternative to the original empirical resuspension function, which was related
 only to the average lake fetch;
- 5) extending the available options for describing light limitation functions for
 <u>individual phytoplankton groups and macrophytes (currently including both an</u>
 <u>integral function based on a Monod-type equation and the original Steele</u>
 <u>equation, which accounts for photo-inhibition (Di Toro and Matystik 1980).</u>

To maintain the integrity of the original PCLake model, in terms of process rates that are formulated on bases of using daily averaged incoming light, we used the ability of FABM to provide daily averaged valuess of photosynthetically active radiation (PAR) for the centre point in any given water column cell. In total, the FABM-PCLake implementation comprises 57 state variables. These include representations of oxygen dynamics, organic and inorganic forms of nitrogen, phosphorus and silicon,
three phytoplankton groups, one zooplankton and one zoobenthos group,
zooplanktivorous and zoobenthivorous fish (representing juveniles and adult fish,
respectively), piscivorous fish and submerged macrophytes (Fig. 1). A complete
record of the partial differential equations for each state variable can be found in the
Supplementary Material.

7 The code implementation involved a complete redesign and rewrite of the PCLake 8 code into a FABM compliant modular structure (see Fig. 2 and Supplementary 9 material, supplementary table S1), thus allowing FABM to acquire sink and source 10 terms for each state variable differential equation, and pass these for numerical 11 solution and transportation by a physical host model. By implementing the model in 12 FABM, one can now combine different ecosystem modules from different 13 biogeochemical models available in FABM to suit the study purpose (such as running 14 the phytoplankton module from the AED model together with the zooplankton module 15 from the PCLake model to simulate the ecosystem for a particular case study). 16 Another important FABM feature is the ability to undertake data assimilation at 17 runtime, where simulated state variables can be "relaxed" to values of observations 18 that are read-in during a simulation. Hereby, one can enforce assimilate certain 19 components (e.g., macrophyte or zooplankton) of the ecosystem with observation 20 <u>data (e.g., macrophyte seasonality)</u>, while simulating other parts of the ecosystem 21 dynamically. The model code was divided into modules of abiotic, phytoplankton, 22 macrophytes and food web dynamics. These modules were further sub-divided into 23 water column (pelagic) and sediment (benthic) domains. Concurrently, we developed 24 an auxiliary module for FABM-PCLake to handle the overall system processes. The 25 overall system processes are the processes that will typically influence several other 26 modules, and they include resuspension, sedimentation and burial. In PCLake, burial 27 is included as a representation of the natural process of sediment accumulation. 28 which is caused by excessive sedimentation (resuspension rate < sedimentation 29 rate) of particles at the sediment-water interface. a process that can prevent a net increase of sediment material by burial of a small layer of sediment, equally thick as 30 31 the layer that had been added to it. The "buried"is material is then considered as 32 buriedinactive in the sediment biogeochemical processes and in the deeper sediment 33 and lostexcluded from the system.

2 3 Model verification

3 To ensure that all biogeochemical processes have been implemented correctly 4 through the equations in FABM-PCLake, we verified the model by running a 5 benchmark test case against the original PCLake model. Hence, we compared 6 output from the original PCLake model (zero-dimensional, using the OSIRIS version, 7 i.e. a C++ executable called from a Microsoft Excel shell) with that from FABM-8 PCLake model executed with a zero-dimensional driver. The models were applied 9 with identical model initialization and parameterization, and the same forcing and 10 boundary conditions in terms of inflow, water temperature, light and nutrient loads for 11 a 5-year period. The initial values for state variables and model parameterization 12 were taken from the original PCLake version, which has been calibrated using data 13 from 43 European lakes (Janse et al., 2010), most of which were Dutch lakes, but 14 also included a few lakes from Belgium, Poland and Ireland. To ensure comparability, 15 we left the Marsh module in the original PCLake model turned off, and used the 16 simple empirical resuspension function (this function remains as an optional function 17 in the FABM-PCLake model, while we also implemented a bottom stress driven 18 resuspension process) in the FABM-PCLake version. Moreover, for the purpose of 19 the benchmark test, processes that are not included in the new FABM-PCLake, such 20 as water column burial correction, dredging and fish harvesting, were turned off in the 21 original PCLake model. We found that there were only marginal differences between 22 the outputs of the two model versions, which could be attributed to small differences 23 in the numerical solvers of the models (Fig. 3). We therefore conclude that the new FABM-PCLake implementation provides corresponding representations of ecosystem 24 25 dynamics, relative to the original PCLake model.

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4 Model features and perspectivesModel applicability, limitations and perspectives

The FABM-PCLake model is now able to run with a selection of hydrodynamic models (which can be simply selected by the user), covering zero-dimensional (included with the FABM source code), one-dimensional (e.g., the General Ocean Turbulence Model, GOTM – http://www.gotm.net, and the General Lake Model, GLM

1 - http://aed.see.uwa.edu.au/research/models/GLM) as well as three-dimensional 2 (e.g., the General Estuary Transport Model, GETM – www.getm.eu, Modular Ocean 3 Model, MOM - http://mom-ocean.org and work in progress - Nucleus for European 4 Modelling of the Ocean, NEMO http://www.nemo-ocean.eu, and The Unstructured 5 Grid Finite Volume Community Ocean Model, **FVCOM** 6 http://fvcom.smast.umassd.edu/fvcom) hydrodynamic models. A major advantage of 7 this development is that the detailed ecological processes provided by PCLake can 8 now be used to study deep and spatially complex aquatic ecosystems. For example, 9 macrophytes was originally represented as a single value in g/m² for a zero-10 dimensional model, but is now able to colonize different depths, for example when coupled to a 1D hypsographic hydrodynamic model, which allows a more gradual 11 12 shift in the ecological states more typical for real lakes, even when shallow 13 (Jeppesen et al., 2007). In addition, it becomes possible to study the concept of critical nutrient loading for spatially heterogeneous aquatic systems. This is important 14 15 because the concept of regime shifts in ecosystems is widely acknowledged in 16 science and ecosystem management, while the effect of spatial heterogeneity on the 17 occurrence of regime shifts is poorly understood (Janssen et al., 2014). Other key 18 features enabled by FABM are:

- 1) the ability to replace one or several of the PCLake modules (e.g.,
 phytoplankton) with that from another ecosystem model available through
 FABM (e.g., ERGOM, ERSEM or AED);
- 22 2) the ability to forceassimilate time series observation data for some state
 23 variables (i.e., data assimilation) while others are left fully dynamic (e.g., one
 24 could force assimilate time series of macrophyte biomass data, and look
 25 atsimulate the response of fish, zooplankton, phytoplankton etc.);
 - 3) the ability to run multiple models in an ensemble (e.g., for inter-model comparisons).
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As we have tried to maintain the overall integrity of the ecological model PCLake,
 some process descriptions may be improved to allow a more conceptually correct
 ecosystem representation in a physically explicit context. For example, higher
 hydrodynamic resolutions (i.e., 1D, 2D and 3D domains), could now allow a more

advanced description of the behavior of macrophytes and fish. One example could
be implementation of a more advanced macrophyte module that could dynamically
re-allocate macrophyte biomass across pelagic grids such as the work presented by
Sachse et al. (2014). Other examples counts potential advances for the fish module,
which could include active fish movement (e.g., through an individual-based model),
or implementation of the foraging arena theory (Ahrens et al. 2012) as adopted in the

- 7 <u>ECOPATH model.</u>
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5 Sample case simulation outputs

10 Whether run as a zero-, one- or three-dimensional model application, the model executable will generate an output file of NetCDF format (*.nc), which can be opened 11 12 and manipulated by a range of software packages (e.g., Matlab, IDL) and a range of free NetCDF viewers, such as PyNcView (http://sourceforge.net/projects/pyncview). 13 14 The latter provides an easy-to-use graphical user interface (GUI) for creation of 15 animations and publication-quality figures. Figure 4 demonstrates (a screenshot of 16 this interface features, with visualization of FABM-PCLake state variables in a 1D 17 context. Output from a one-year case simulation of temperature and macrophyte depth profiles is shown in Figure 5. This output was produced by linking FABM-18 PCLake with the 1D GOTM model (including a hypsograph that describes the 19 20 relationship between depth and sediment area) for a hypothetical temperate 20m deep lake (with default PCLake parameterization). is demonstrated in Fig. 4). 21

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24 Code availability

The model can be compiled and executed on Windows, Linux, and Mac OS machines, and is open source and freely available under the GNU General Public License (GPL) version 2. Source code, executables, and test cases can be downloaded directly from http://fabm.net, or as git repositories (updated information on how to download the code from git repositories as well as compiling the code for different platforms is available from the FABM wiki at http://fabm.net/wiki). Contact persons for FABM-PCLake model: Fenjuan Hu (fenjuan@bios.au.dk), Dennis Trolle (trolle@bios.au.dk), Karsten Bolding (bolding@bios.au.dk). Contact persons for the
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Fig. 1. Conceptual model of FABM-PCLake (FABM, Framework of Aquatic biogeochemical Models; PCLake, the implemented aquatic ecosystem model). Key state variables of the FABM-PCLake biogeochemical model and the interactions
between these (represented by arrows); and an illustration indication of how a physical model may now transport biogeochemical state variables through explicit physical processes.



Fig. 2. The modular structure of the FABM-PCLake code. Each square box 3 represents a FORTRAN module of FABM-PCLake (and these modules are 4 5 interacting/communicating through FABMto simulate the processes illustrated by 6 arrows in Fig.1). The brown coloured boxes are related to the sediment domain and 7 the blue boxes to the water column domain. Note that all modules may be applied for 8 0-D to 3-D spatial domains. A detailed description of the contents of each module is 9 provided in the Supplementary Material.



Fig. 3. Key time series outputs from a five-year simulation by the original PCLake
model (PCLake-Original), and the new FABM-PCLake model (FABM-PCLake),
represented by dry weight of total phytoplankton biomass, dry weight of zooplankton
biomass, dry weight of macrophytes biomass, and the concentration of phosphate in
the water column.



Fig. 4. Visualization of FABM-PCLake state variables in PyNcView, exemplified by a two yeartwo-year period simulated by a one-dimensional FABM-PCLake application of a 20 m deep water column. State variables to be viewed are simply selected in the left panel, and figures can be viewed, manipulated and saved in the right panel and as detached figures (a detached figure is exemplified by the temperature plot).

