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Blueprint for a unifying framework for synthesis of aquatic ecodynamics

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Abstract: Quantitative assessments of aquatic ecosystem dynamics and services are required to guide decision support activities and assess how socioeconomic scenarios of human development impact our aquatic environment. However, we are poorly equipped to predict across a broad range of scales the physical, biogeochemical and ecological interactions that control carbon and nutrient flux pathways, despite a plethora of models and model approaches that have emerged. Our models have languished due to ambiguities and lack of agreement in model conceptualisations, a focus on point-scale rather than system-scale validation, and a general inability to deal with uncertainty, particularly in spatially-resolved inter-disciplinary models. Further, the site-specific and highly disciplinary nature of many model applications limits synthesis and transferability of knowledge between sites. Here we outline a blueprint for an integrative approach to address these barriers by facilitating: *i)* the integration of inter-disciplinary modelling approaches, *ii)* reducing uncertainty through a multi-scale validation approach and managed assimilation of environmental sensing data, and *iii)* cross-domain synthesis.

***Keywords**:* biogeochemical model, synthesis, data assimilation, aquatic systems.

1 INTRODUCTION

1.1 Understanding aquatic ecosystem response to disturbance

Aquatic systems are under pressure from altered hydrological regimes, invasive species, eutrophication and pollution from contaminants, which together degrade ecosystem services, reduce biodiversity, and negatively influence human health. The implications of future global change scenarios on aquatic ecosystems are "staggering" [Mooney 2010], and may amplify these degradation processes. In general, ecosystems are vulnerable to deterioration when key system functions are pushed over thresholds, resulting in the loss of resilience and the emergence of a regime shift. Indicators used to assess resilience and regime shifts are generally related to biodiversity, but cycles of carbon and nutrients (generally nitrogen and phosphorus) underpin resource partitioning, organism dynamics and ecosystem function. There is an extensive body of literature describing theory around ecosystem stability and resilience to disturbance [eg., Scheffer et al. 2001; Jeppesen et al. 2005] that can be summarised in the context of aquatic systems by stating that they are characterised by: i) inertia and resilience in largely unimpacted states, ii) thresholds and tipping points in response to disturbance, and iii) impacted, resilient states that lack integrity, diversity and serve poorly in provision of ecosystem services. Only conceptual models, idealised field experiments, and rudimentary numerical models have been used to tell us anything about these dynamics. Understanding how they manifest in complex real-world systems is ultimately required, as are tools to holistically assess how land-use change, river-basin engineering and climate variability combine to affect water quality and biodiversity. The main challenge in exploring these dynamics in complex landscapes is the inherent spatial heterogeneity and highly dynamic nature of resource pathways (eg., transport processes and biogeochemical pathways). Spatial patterns and diversity in ecosystem attributes play a crucial role in shaping function and resilience, seen across the continuum from individual organisms up to whole landscapes [van Nes and Scheffer 2005a; Kratz et al. 2007]. Further, we must consider that real-world landscapes are comprised of networks of aquatic ecosystems that link together (eg., wetlands, rivers, lakes, estuaries). Connectivity is critical in shaping habitat and patterns of resource flow, by regulating the transfer of water, energy, organisms and elements. Each sub-system in a river basin network has a different ability to process carbon and nutrients and the characteristic biogeochemical pathways [Harris 1999]. If we consider that humans have influenced aquatic ecosystem connectivity more than almost any other ecosystem attribute through river-basin engineering [Nillson et al. 2005], we must also understand how changes in connectivity manifest in system scale dynamics, such as resilience and stability, and how they combine with other stressors to potentially lead to undesirable regime shifts.

1.2 The need for integration and synthesis

To quantify the carbon and nutrient flux pathways requires the synthesis of a vast array of information across numerous discipline areas, and necessitates an improved, integrative, modelling framework to predict how patterns of water, carbon and nutrients translate across the range of scales found in river basins. Our aim in this paper is to explore the different dimensions of this problem and describe a blueprint for such an integrated approach. The discussion focuses around bringing together recent technological advances in models of aquatic biogeochemistry, environmental sensing techniques, and the associated ‘cyber-infrastructure’ in a way that balances process-driven and data-driven approaches for exploring ecosystem function.

2 CHALLENGES IN MODELLING AQUATIC BIOGEOCHEMISTRY

Models of catchments, lakes, wetlands, rivers, estuaries and the coastal ocean are now widespread for simulating water quality response to change and to unravel nutrient pathways. Their growing importance is evidenced in the sharp rise in the number of published applications in the literature [Trolle et al. 2012]. They are used as ‘virtual environmental laboratories’ for developing ecological theory and to study feedbacks and sensitivities of particular sites in response to changes in natural forcing or through their interface with human systems [van Nes and Scheffer, 2005b]. Coupled physical-biogeochemical-ecological models are used to unravel how key biogeochemical pathways are superimposed on a dynamic physical environment that responds to hydrologic forcing, wind mixing, tides etc..

But how do they perform in the context of addressing the science challenges as outlined? In general terms, despite considerable advances and the numerous model platforms that are now available, it remains difficult to simultaneously predict pathways of water, carbon and nutrients through complex landscapes, and therefore to understand how the pathways and interactions scale-up to manifest in ecosystem-scale response to change [Mooij et al. 2010]. In particular, it is argued that despite improved process understanding of eco-physiology, biogeochemical processes and trophic interactions in the experimental literature, models have failed to keep up, and remain highly disciplinary [Flynn 2005], and widely criticised for failing to reign in uncertainty [Arhonditsis et al. 2008]. To apply models to assess how complex systems respond to disturbance, Mooij et al. [2010] highlighted several barriers that must be overcome:

i) *Ambiguities in model conceptualization has led to a plethora of models and approaches*: A major barrier is the simple practical aspect that there are lots of models and model approaches, but limited open-source codes and standards that bind the community or facilitate integration. To solve complex inter-disciplinary problems flexibility is required to integrate diverse approaches and bring together those with different strengths and those that span across relevant scales.

ii) *Difficulty in linking between biogeochemical models of diverse aquatic systems*: Whilst we have excellent fixed-dimensional model platforms for simulating aquatic environments, for example, the Computational Aquatic Ecosystem Dynamics Model (CAEDYM), which is coupled to 1D & 3D hydrodynamic models [Hipsey et al. 2007a], the questions being asked range across management issues at river basin scale. We must therefore be able to consider inter-connected rivers, lakes, estuaries and even extend to cover the coastal impacts.

iii) *Managing uncertainty in complex models is difficult*: Aquatic system models that unravel the effects of spatial heterogeneity are inherently multi-dimensional and contain extensive sets of linked equations that govern the interactions of key components (nutrients, primary producers, etc.) from the scale of a numerical 'cell' to that of the whole domain. However, to date the community has relied on testing model performance at point scale and it generally remains unclear whether the constitutive equations, which are mostly based on laboratory or plot-scale relationships, come together to successfully capture system-scale feedback mechanisms, the degree of ecosystem stability and resilience, and general response pathways to change. The introduction of procedures to validate model performance against metrics that characterise ecosystem-scale response pathways will improve model confidence to capture such behaviours.

3 BLUEPRINT FOR A UNIFYING APPROACH

The approach described here is designed to over come the above barriers since the current fragmented and disciplinary approach prevents synthesis. The concept of 'model-data fusion' is increasingly being seen as a means to manage model uncertainty and premised on the notion that we must accept that uncertainty is inevitable in our complex ecosystem models. The 'assimilation' of data from both remote and in-situ sensors using data-driven analysis techniques can be used to identify and manage model error, ie., 'model adaptation' [Hipsey et al. 2007b]. Developments in sensing technologies, both in-situ probes and remote sensing products, and the accompanied progress in cyber-infrastructure and computational techniques for data analysis [Hanson 2007; Porter et al. 2009], have created new opportunities for understanding how systems respond to change and they cover an unprecedented range of spatial and temporal scales. For example, Tsai et al. [2011] has demonstrated the benefits of data assimilation and inverse modelling techniques from in-situ sensors for extracting meaningful information on ecosystem carbon metabolism and lake resilience. Spatial analysis of water quality variables using satellite imagery is also now routinely performed, and methods have emerged for their integration with model assessments [Liu and Woods 2004].

These advances provide new opportunities to deal with issues of model uncertainty in addressing the science challenges, by allowing us to maintain model validation against multi-scale ecosystems metrics, thereby ensuring errors are not cumulative and do not become amplified along the modelled hydrological landscape. Here we attempt to outline an integrative approach. The framework is built on three fundamental building blocks – each of which supports a context specific level of integration. Whilst the vision presented here is far-reaching, we propose a general framework that combines the overall vision with practical and tangible steps that can serve as a blueprint to focus our development (Figure 1).

3.1 Community code & standards: *Disciplinary integration*

Our analysis requires flexibility to join a range of coupled models of hydrodynamics/hydrology, biogeochemistry and aquatic ecology. Spatial dimensionality and system compartmentalisation must be addressed as we require a diverse array of physical drivers (eg., wetland/floodplain model, river model, lake model, estuary model) to couple with biogeochemical / ecological 'components'.

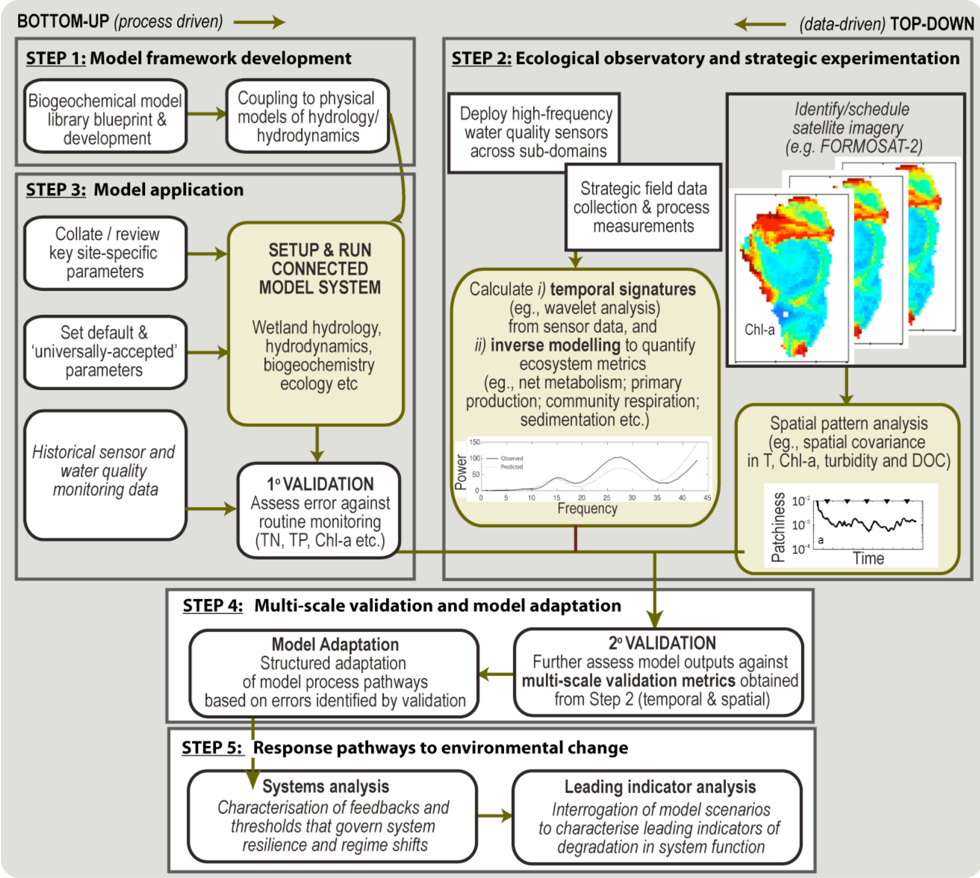

Figure 1. Summary of framework outlining the sequential development of the integrated approach.

Model typology and numerical framework: *flexibility to deal with complexity*

Definition of an architecture of the key numerical and software elements to facilitate and harmonize development efforts. An outline of the concept [Trolle et al. 2012] has been developed as a collaboration of the Aquatic Ecosystem Modelling Network (AEMON), and progress has been made through development of the Framework for Aquatic Biogeochemical Models (FABM). Each model object focuses on a key ecosystem component (e.g. nutrients, phytoplankton, organic matter, macrophytes, emergent vegetation, sediment), and cross-module dependencies are setup such that the many hundreds of derivatives for the kinetic production and destruction terms of the biogeochemical equations are easily managed for numerical solution by a collection of Ordinary Differential Equation (ODE) solvers (e.g. Burchard et al. [2005]). In addition to the main water column processes, detailed benthos and sediment biogeochemistry modules exist, and options for simulating geochemistry (equilibrium speciation, redox processes and precipitation/dissolution) also exist.

Importantly, the proposed approach does not mandate a particular model but rather a community library that serves as a collection of flexible model objects that can be used within custom system idealisations based on their own scientific reasoning. Complex models require a suitable level of observational data for validation, which is not always available to provide a necessary level of validation. Instead, our approach acknowledges that ecosystem complexity is often paramount in shaping dynamics, but that we are constrained by the need for testable models. Therefore, a structured approach to gauge complexity requirement is necessary, and flexibility in our model formulation and integration approaches must be factored in to deal with complexity. The approach also encourages multiple model comparisons and ensemble model predictions.

Coupling interfaces to physical drivers: *accommodating diversity*
Since there will be multiple physical models (and grid types) necessary to cover the diverse scales of interest, we must accommodate a generic approach where processes in the above library are 'split' to separate the components dealing with transport and mixing, and those dealing with reactions and transformations, etc.. This approach has been used in various contexts, however to deal with the complexity of networks of aquatic environments and the terrestrial–aquatic interface, deeper consideration of integration of model approaches is necessary. Trolle et al. [2012] outlines these requirements and a specification for FABM.

Standards for model application and development: *comparing apples with apples*
To date, there have been limited standards in aquatic models [Schmolke et al. 2010]. To facilitate cross-site comparisons – as is required for synthesis – it is necessary for similarities in approach [Robson et al. 2008], and also a requirement to develop a common nomenclature and vocabulary.

3.2 Model-data fusion: *Methodological integration*

Mixed modelling: *playing nicely with others*
As identified above, there is little crossover between model approaches such as linking complex dynamic models with individual based models, however the utility of such a mixed modelling approach has been recently demonstrated by Makler-Pick et al [2011] and the benefits of which are discussed in Mooij et al [2010]. This idea can be taken further, by considering the fusion of 'top-down' and 'bottom-up' approaches within a coordinated/flexible system, that allows for mixed-modelling approaches. For example, 'bottom-up' (deterministic) approaches can be used to improve our understanding of the physical, chemical and biological roles on water quality and habitat dynamics, but where attempts are made to resolve the higher ecological interactions between more complex organisms or communities, a lack of suitable validation data and excessive model complexity in the absence of guidance by sound empirical data hinders progress and often means that higher trophic levels are ignored. Point scale (rather than system scale) validation also means that it generally remains unclear whether all important ecosystem feedback mechanisms are represented. These fundamental limitations can have a profound impact on their ability to predict responses to environmental change, and whether 'emergent' ecosystem behaviours (patterns that emerge due to complex system dynamics) such as those observed in nature can be resolved. Ecosystem ecologists, however, have a long tradition of innovating models to fit the science questions and observational data characteristics using 'top-down' (data-driven) modelling approaches. Computational demands typically are low, allowing for rapid model evolution and exploration of uncertainty through a range of analysis methods. The opposite problem exists here owing to the highly aggregated nature of these models, which inherently means that many processes are lumped in space and time, precluding discrimination among the underlying mechanisms. New knowledge can be discovered through tight interactions between data based and deterministic approaches - top-down modelling can validate and inform bottom-up modelling, and vice versa, in a feedback loop, to ultimately result in a more comprehensive understanding of aquatic system response to perturbation. Whilst lip service is often paid to bringing together top and bottom approaches, practically it remains a challenge, and further development of approaches to integrate such methods are required, such as those outlined next.

Multi-scale validation and model adaptation: *learning from our mistakes*
Our model approach must adopt more rigorous procedures for validation of patterns and processes. In the proposed framework we outline that the model must

be initially validated ('1° validation') against measured physico-chemical sensor and profile data, biogeochemical and ecological data from the range of monitoring sites across the domain. This can come from our sensor networks or data from routine monitoring programs and follow conventionally accepted procedures for model performance assessment.

Ideally, model fidelity should be tested not only against variables, but also against fluxes and rates of material flow. The novel aspects within this framework is the requirement for assessment of model performance across a continuum of spatial and temporal scales, and against ecosystem patterns and processes ('2° validation'). Use of data assimilation routines to extract key information from relevant observational data using inverse modelling approaches (eg., photosynthesis and respiration rates derived from oxygen data, as per Hanson et al. [2008]; water column mixing as per Read et al. [2011]), and signal processing techniques such as wavelet transforms on data series (eg., see inset in Fig. 1, Kara et al. [2012]) to characterise representative multi-scale signatures is one pathway to reduce uncertainty. Assessment of spatial patterns in temperature, Chl-a, DOC and turbidity from satellite images by assessing spatial covariance and 'patchiness', and other metrics for assessing phytoplankton growth from images [Liu and Woods 2004] proved a second pathway. Further detailed process pathway validation can be done by assessing resource partitioning within trophic pathways against isotopic and stoichiometry data. In summary - aside from routine validation assessment against key variables, a major component of the framework is also to validate the model against higher-order ecosystem signals, patterns and processes across a continuum of different temporal and spatial scales

Uncertainty in model predictions is inevitable and we expect a complex model such at that proposed here to show mixed performance based on the traditional (1°) and detailed validation (2°) conducted above. Within the framework we can extend our approach by accommodating managed validation by combining top-down and bottom up methodologies, guided by performance across the multi-scale assessment. This would entail managing model performance by dynamically adjusting key parameters during the simulation in response to detailed empirical analysis of sensor network and satellite data. This has been reported for improving surface water stratification predictions [Yeates et al. 2008], but further development is required to allow carbon and nutrient variables to also be able to be updated. As an example, for primary productivity, it is possible to firstly derive the photosynthesis rates empirically from continuous T and DO data (eg., using the approach of Hanson et al. [2008]), and compare against the model equivalent process rate, whilst also assessing spatial variance within satellite images, and compared to spatial patchiness in model predictions. Following a combined assessment of these, relevant model parameters (eg., growth or vertical migration rate) can be gradually adjusted to bring the predictions back in line with the observations. Further opportunity exists to examine the history of model errors and parameter values using data-driven informatics procedures to explore the drivers of the recorded uncertainty.

<u>Incorporating models within sensor networks: *hybridising our models*</u>
Over the past decade, not only have our sensors, computational techniques, and developments in models and our core scientific understanding of aquatic processes advanced considerably, but also the cyber-infrastructure and hydro-informatics tools available to us has also grown rapidly. These tools serve as the glue to bring together and 'hybridise' our numerical models and observational resources (Figure 2) and ultimately will accelerate model advancement.

3.3 Cross-domain synthesis: *Geographic integration*

Synthesis activities must aim to search for universal descriptors of process, commonality in ecosystem emergent behaviours, and specifically how patterns in carbon and nutrient pathways vary across geomorphologic and climate gradients.

Quantitative information on resource flux pathways and higher-level ecosystem pattern and process information from diverse model applications should be extracted over different scales of integration to support cross-domain comparative analyses. While simple in theory, in practice this is a challenge due to lack of standards and common approaches. The emergence of 'network science' is able to foster a community approach and encourage such cross-site comparisons. An example of embedding model systems within a global water resource observatory network (GLEON, cdi.gleon.org; Figure 2) demonstrate this is possible.

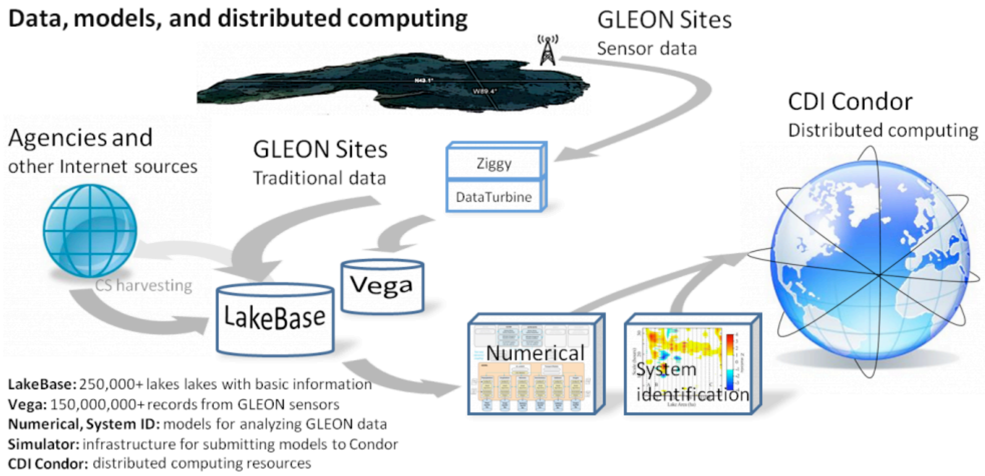

Figure 2. The 'cyber-infrastructure ecosystem' developed by the Global Lake Ecological Observatory Network (GLEON) for integrating data sources and models.

4 CONCLUSION

The approach aims to advance understanding of the complex linkages between water flow, carbon and nutrients concurrently across a large range of spatial and temporal scales, and diverse aquatic environments. We introduce the use of ecosystem-scale measures of function and resilience for providing more robust assessments of model predictions. The adoption of community models and implementation of data-driven modelling approaches to validate and reduce error in spatially-resolved mechanistic models, will ultimately lead to more robust assessments of aquatic systems. Specifically, the approach can support our understanding of 1) the multi-scale dynamics of nutrient flux pathways in complex real-world systems; 2) how ecosystem connectivity, that is the timing and magnitude of water and resource flows between connected sub-systems, influences nutrient flux pathways; and 3) how resilient the dominant biogeochemical pathways are to changes in hydro-climatology and other anthropogenic changes, and thresholds where they are altered to an extent that the functionality and resilience of the system is reduced.

The blueprint outlined in this paper promotes synthesis by integrating diverse models in a way that balances process-driven and data-driven approaches for exploring ecosystem function. Importantly, these developments are not in isolation, but rather must be facilitated through development of an active community of developers and users that encourages comparative analyses. It is therefore envisioned that, while not all sites are able to adopt the framework in full due to a lack of data, the general advances made by the community will continue to underpin our ability to apply models for decision-support of data-poor systems.

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