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Key Points:

- New demands are being made for aquatic ecosystem prediction
- We outline a framework for model use within environmental observatories for aquatic systems
- Improved model systems able to predict ecosystem services can better support management

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Predicting the resilience and recovery of aquatic systems: A framework for model evolution within environmental observatories

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Abstract Maintaining the health of aquatic systems is an essential component of sustainable catchment management, however, degradation of water quality and aquatic habitat continues to challenge scientists and policy-makers. To support management and restoration efforts aquatic system models are required that are able to capture the often complex trajectories that these systems display in response to multiple stressors. This paper explores the abilities and limitations of current model approaches in meeting this challenge, and outlines a strategy based on integration of flexible model libraries and data from observation networks, within a learning framework, as a means to improve the accuracy and scope of model predictions. The framework is comprised of a data assimilation component that utilizes diverse data streams from sensor networks, and a second component whereby model structural evolution can occur once the model is assessed against theoretically relevant metrics of system function. Given the scale and transdisciplinary nature of the prediction challenge, network science initiatives are identified as a means to develop and integrate diverse model libraries and workflows, and to obtain consensus on diagnostic approaches to model assessment that can guide model adaptation. We outline how such a framework can help us explore the theory of how aquatic systems respond to change by bridging bottom-up and top-down lines of enquiry, and, in doing so, also advance the role of prediction in aquatic ecosystem management.

1. Modeling Aquatic Health: The Evolving Role of Aquatic System Prediction

Sustainable catchment management during the current era of global population growth and climate change is one of the most profound challenges confronting society [*Bogardi et al.*, 2012; *Gerten et al.*, 2013; *Pahl-Wostl et al.*, 2013; *Brookes et al.*, 2014]. Inland waters have changed more rapidly in the past 50 years than at any other time in human history. Water quality degradation and associated issues of water security, as well as loss of biodiversity [*Vörösmarty et al.*, 2010; *Dudgeon*, 2014], have been driven by widespread urban, agricultural and mining developments, and span both developed and emerging economies. Preserving the integrity of aquatic systems, including rivers, wetlands, lakes and estuaries, is an essential component of catchment management as these systems provide critical ecosystem services to support societal development [*Zedler and Kercher*, 2005; *Carpenter et al.*, 2011]. However, the pace of contemporary environmental change is rapid and multifaceted, and hinders restoration efforts. The development of tools and approaches to quantify the function and response of aquatic systems is therefore essential to support a holistic view of catchment function [*Wagener et al.*, 2010; *Montanari et al.*, 2013], and guide investment in conservation and rehabilitation [*Creighton et al.*, 2015].

Substantial advances have been made toward describing changes in catchment hydrologic function and developing predictive ability to support water resource management [*Blöschl et al.*, 2013; *Vrugt and Sadegh*, 2013]. However, the challenge of prediction becomes significantly more complex as we broaden our scope to consider water quality, and even more formidable as we attempt to consider the "health" of aquatic environments in entirety. We refer to health here as the ability of ecosystems to maintain their ecological function and biodiversity, but also include in this definition the provision of ecosystem services such as drinking water, recreation and amenity opportunities, and productive freshwater and estuarine fisheries [see *Costanza and Mageau*, 1999 for a discussion on what health refers to].

A diverse suite of models to simulate water quality and aquatic system function has emerged in response to this challenge. Two recent special issues [*Arhonditsis et al*., 2014; *Gal et al*., 2014 and papers therein] were dedicated to describe the progress in and challenges for these model communities. They highlight the progress that has been made in terms of the diversity of approaches, expansion in process complexity and spatial resolution, as well as technical advances in model integration and uncertainty assessment. On the other hand, they also point to limitations in model performance, challenges in integration and issues when scaling predictions up to capture system responses, as well as the difficulty in simulating higher-level biota [e.g., *Heathwaite*, 2010; *Robson*, 2014b]. Ultimately, the challenge that confronts us is how can we advance models so they are able to quantify and integrate dynamics of aquatic systems based on the symphony of local (e.g., engineering), regional (e.g., environmental flow regimes and water trading), and global (e.g., climate variability) pressures and thereby meaningfully inform policy. One of the more difficult questions increasingly being asked of models is to estimate the level of impact that may trigger abrupt transitions or regime shifts in ecosystem state, or alternatively, to describe the effort required either to avoid adverse transitions or to restore degraded systems back to some "acceptable" level of structure and function [*Rockström et al*., 2014]. Continued effort is therefore required to build the next generation of modeling tools capable of predicting the diversity of attributes that contribute to aquatic system health across the range of temporal and spatial scales relevant to decision making.

No single new model is going to meet this challenge. Modeling aquatic environments across broad and heterogeneous landscapes requires rich streams of data [e.g., *Porter et al*., 2009; *Read et al*., 2014], and the level of process-complexity and interdisciplinarity required to simulate the multiple attributes of system function across a range of scales demands effective science teams [*Cheruvelil et al*., 2014] able to foster the integration of diverse perspectives [e.g., *Ehret et al*., 2014]. The emergence of integrated environmental observatories that combine sensor and model infrastructure, in conjunction with human networks, has offered benefits in terms of improving how we undertake predictions, and this is shifting how models integrate with the decision-making process. However, to meet the demands on prediction that are outlined above, a suitable framework for model integration and learning within observatories is required that considers both technical (e.g., data assimilation procedures) and theoretical (e.g., capturing system resilience) aspects of model operation.

This paper therefore aims to address two questions: (a) how well can we model the health of aquatic systems and what are the limits of our predictive ability, and (b) how can we better integrate diverse model approaches with the expanding repositories of observations emerging out of advances in sensor networks? The analysis is structured to first explore specific challenges associated with modeling aquatic ecosystem health in terms of process complexity and scale (section 2). In section 3, we focus on identifying the needs and abilities of models to simulate ecosystem resilience to multiple stressors. We then propose in section 4 that careful integration of flexible model libraries with data from observation networks within a learning framework can serve to more efficiently link empirical and mechanistic lines of enquiry and facilitate improved use of models for decision-making. Finally, we highlight in section 5 the importance of science teams for bridging the gap between technical and theoretical developments, and suggest community level initiatives required to accelerate model development and synthesis activities.

2. Model Diversity and Challenges for Prediction

Simulation of aquatic system health requires the integration of models of hydrology, hydrodynamics, biogeochemistry, and ecology. There are two broad categories of models that have emerged [*Arhonditsis et al*., 2014]: (1) catchment-scale water quality models and (2) aquatic biogeochemical models applied to individual systems within a catchment (e.g., wetlands, lakes, large river domains, and estuaries). These two categories can be further subdivided based on the diversity of modeling approaches, demonstrating the broad range of scales and disciplinary foci covered by the models (Figure 1).

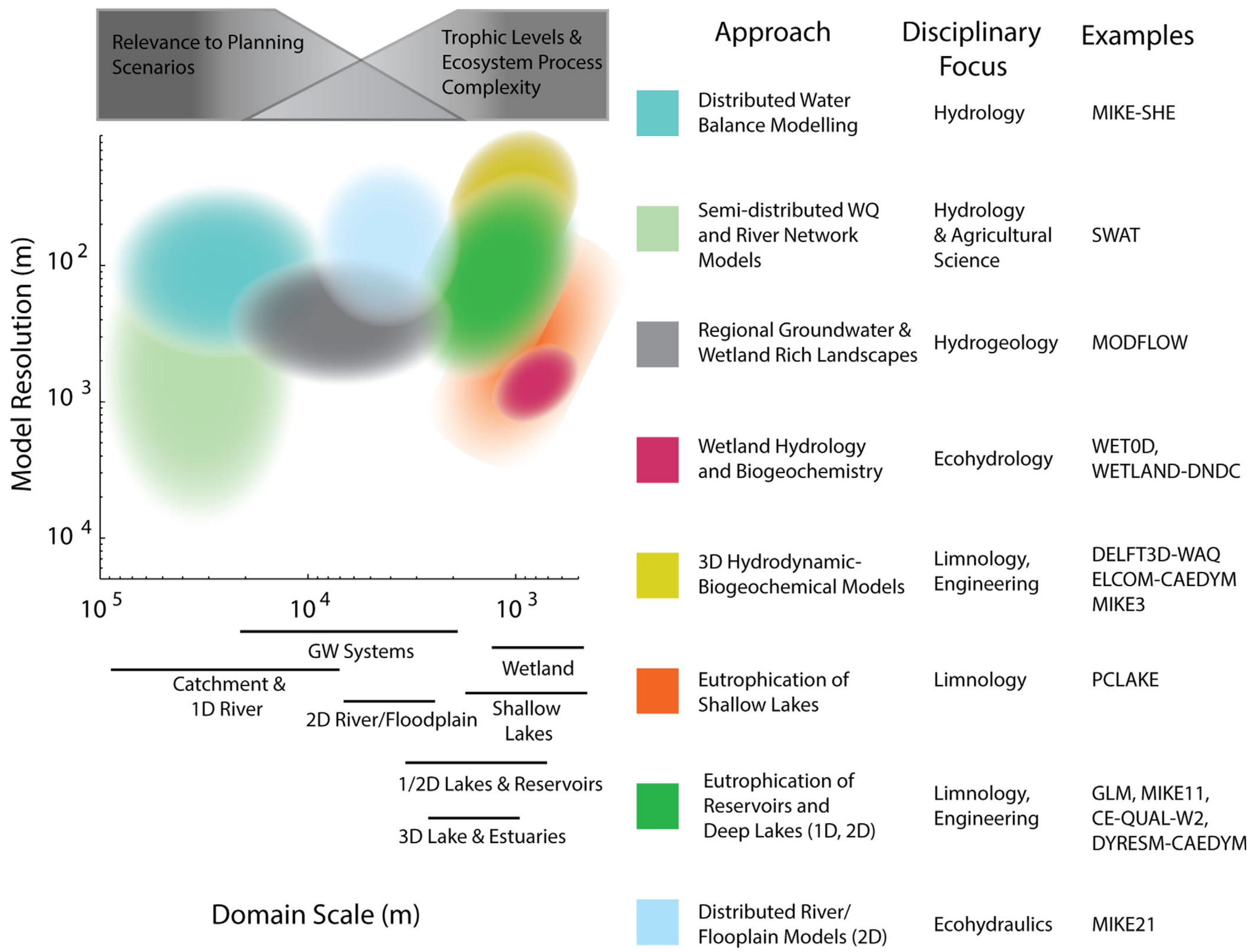

Figure 1. Conceptual overview of the spatial extent of simulation domains and indicative numerical resolution used by a range of disciplines to simulate aquatic ecosystem responses to change. A nonexhaustive list of examples of models used to simulate these domains is presented in the right-hand column.

As these models are increasingly used to make predictions about aquatic health and ecosystem services, integration across scientific disciplines is necessary, however, there is often divergence in modeling philosophy, spatiotemporal scale, and computational methods since various model approaches have historically evolved within well-defined disciplinary boundaries. When aiming to develop an integrated predictive capacity to broadly inform catchment policies, amplification of model complexity is inevitable, yet a question that modelers are often confronted with is, "what level of spatial resolution and model complexity is required to adequately simulate the impacts of multiple stressors?" This section therefore explores the capabilities and limits of our models to compute the multiple ecosystem attributes relevant to ecosystem health, considering issues of process complexity, scale, and model integration.

2.1. How Much Complexity Is Enough?

Historically, water quality models were developed to answer relatively simple questions related to the response of water column nutrient, oxygen, and chlorophyll-a concentrations to changes in nutrient loads and hydrology. These proved to be effective tools for supporting the introduction of nutrient reduction targets, but often performed poorly in simulating variability in key water quality parameters [*Arhonditsis et al.*, 2006]. The increase in resolution and quality of our observational data has since facilitated the development of more complex models that now incorporate a greater number of biogeochemical variables and processes, and this has enabled more specific questions to be addressed, such as the role of sediment storage and release of nutrients [*Paraska et al*., 2014] and the interaction of multiple biotic groups [*Robson*, 2014a]. In particular, for the case of coupled physical-ecological aquatic models, the focus of advancing process descriptions has been on enabling the simulation of multiple phytoplankton and zooplankton functional groups [*Li et al*., 2013; *Chung et al*., 2014; *Reynolds et al*., 2014], capturing stoichiometric variability and improving descriptions of microbial interactions such as the microbial loop and viral shunt [*Keller and Hood*, 2013; *Li et al*., 2014]. The importance of considering food quality for grazers has also been recently highlighted, with indications that capturing the internal stoichiometry [*Li et al*., 2014] and fatty acid concentrations [*Perhar et al*., 2013] of their prey is necessary to accurately resolve nutrient transfer within the food web and the pattern of phytoplankton succession. These advances have improved our ability to predict the occurrence of nuisance algal blooms, however, some shortcomings remain, for example our ability to simulate algal toxins. Simulation of aquatic geochemistry and contaminants that present an ecosystem or human health risk has also advanced considerably, including models for pathogens [*Hipsey et al*., 2008], metals, and organic contaminants [*Gandhi et al*., 2011, 2014], acidity [*Hipsey et al*., 2014], and hydrocarbons [*Perhar and Arhonditsis*, 2014].

Complexity is often paramount in shaping ecosystem dynamics, depending on the specific question being addressed, but models by necessity are some simplification of reality. The aquatic modeling community has developed model packages that span the diversity from simple to complex (Janssen et al., Exploring, exploiting and evolving diversity of aquatic ecosystem models: a community perspective, *Aquatic Ecology*, in review), with the consequence that a plethora of approaches and packages have emerged, each with differences in model conceptualizations, implementation, and parameterizations. Whilst this diversity is a sign of an active and creative community exploring models of varied complexity, applications remain largely heuristic [*Arhonditsis et al*., 2014], and uncertainty remains in terms of identifying clear limits of predictability of specific approaches, i.e., for any given question how much complexity is "enough"?. For example, it may be the case that a simple single-layer sediment biogeochemical model is adequate to capture the long-term changes in internal nutrient loading within an urban river system, whereas a vertically resolved sediment diagenesis model may be required to accurately resolve the impact of water level manipulation on greenhouse gas emissions from a hydropower reservoir. Similarly, how many phytoplankton should be simulated to accurately predict the risk of a particular harmful algal species blooming?. A handful of studies have been undertaken to highlight the importance of carefully choosing model structural complexity [e.g., *McDonald and Urban*, 2010; *Paudel and Jawitz*, 2012; *Li et al*., 2014], however, further synthesis is required to facilitate the development of clear guidelines able to recommend what level of complexity is necessary to achieve adequate predictions given a particular application context. By defining the essential environmental attributes that govern changes to the key ecosystem services relevant to decision-making as a target for prediction, we may ultimately help the research community better focus effort on defining when models are able to capture the dynamics of the system without being overly complex.

2.2. Modeling Food Webs and Higher Biota

The usefulness of models to support a holistic assessment of aquatic systems is increased greatly when trophodynamic relationships and trends in key biota (e.g., vegetation, bivalves, fish) are included. Models of lakes and estuaries have tended to have more sophistication in terms of trophic complexity than catchment and river network models (Figure 1), although predictions of biotic responses across river basin scales have been demonstrated [e.g., *Wells and Wells*, 2012; *Van Looy et al*., 2014]. Predicting biotic responses for the purpose of assessing ecosystem health requires the integration of models of hydrology/hydrodynamics, biogeochemistry, and biotic interactions. Integrating aquatic biogeochemical models with individual-based modeling approaches has been undertaken for fish and mesozooplankton [*Makler-Pick et al*., 2011] as well as bivalves [*Bocaniov et al*., 2014; *Gudimov et al*., 2015] and macrophytes [*Li et al*., 2010]. However, confidence in predictions is reduced significantly beyond phytoplankton [*Arhonditsis and Brett*, 2004], and new efforts are required to bridge the gap between physical-biogeochemical models and ecosystem food-web models [*Harris and Heathwaite*, 2012]; a challenge similarly faced within the marine ecosystem modeling community [*Mitra et al*., 2014].

Nonetheless, it is possible to develop predictions of habitat quality and biotic health relevant to our decision-making needs through integration with empirical model approaches from the extensive ecological literature on environmental-faunal linkages [*Shallin Busch et al*., 2013]. For example, rather than explicit simulation of biotic populations in the benthos, simulation of simple habitat metrics known to drive population abundance may suffice in many applications. Capturing their feedback onto the overlying water quality (e.g., dissolved oxygen, turbidity, and nutrients) may be possible with relatively simple parameterizations (e.g., bioturbation, sediment stabilization, etc.). Therefore despite uncertainty in simulating population dynamics, for the purposes of capturing the role of biota on aquatic system health for scenario investigations, there is scope to combine statistical environmental-faunal relationships with dynamic models that are able to competently simulate key habitat properties.

2.3. Modeling Across Scales

Spatially lumped models are often used to explore system-level responses to environmental change, however, it is well-documented within the ecological literature that variability across the continuum from individual organisms up to entire ecosystems can play a crucial role in shaping function and resilience [*Pimm*, 1984; *Kratz et al*., 2005; *van Nes and Scheffer*, 2005]. Model studies have advanced to demonstrate more clearly the scale of resolution that is required to resolve the inherently important dynamics of aquatic systems. For example, in lake environments it has been demonstrated that spatial "patchiness" that emerges due to the circulation dynamics can shape the distribution and intensity of phytoplankton blooms [*Wynne et al*., 2010; *Michalak et al*., 2013; *Chung et al*., 2014], with 1-D and 3-D simulations giving quite different predictions of phytoplankton distributions even if all other model aspects are equal [*Hillmer et al*., 2008; *McDonald et al*., 2012]. Thus the degree of model resolution may be tailored to address the scale of the question. For example, simulating hypolimnetic oxygen depletion within a large reservoir may be adequately modeled with a horizontally-averaged model, but in the same system, prediction of the risk of cyanobacterial blooms may in fact demand 3-D resolution to capture patchiness and the emergence of niches. As a further example, avoidance behavior of fish to hypoxia in feeding zones can lead to a long-term shift in abundance and body condition of the population [*Cottingham et al*., 2014], which would be challenging to predict without a model able to resolve habitat heterogeneity. Whilst modelers already pay attention to these issues, decisions on model resolution are often ad hoc since there are no defined limits of predictability of models with different spatial dimensionality. Furthermore, the necessary level of spatial resolution required may in fact vary depending on the underlying conditions and time-scale of the simulation. In an ideal case, integrated model systems would allow for flexible model domain resolution that would be able to be enhanced or reduced as required in order to adequately account for effect of spatial variability on ecological function. However, poor understanding of the scaling of parameters and parameterizations in models, to account for the degree of spatial aggregation, has made the interchangeability of models that have similar biogeochemical conceptualizations but different physical process resolutions difficult.

Choice of model resolution and approach becomes more challenging with progression from individual aquatic systems to interconnected networks of aquatic systems within a catchment (Figure 2). Recent efforts in model integration have facilitated the coupling of catchment and aquatic system models (Figure 2a) to explore the impacts on large water bodies of catchment nutrient reduction plans and restoration initiatives [*Waltham et al*., 2014; *Kim et al*., 2014a], and allow for prediction of aquatic system health under future climate change projections [*Cloern et al*., 2011]. These whole-catchment applications are promising, but there is ongoing need to refine individual constituent models of the system including within-stream and hyporheic processes [*Hattermann et al*., 2006; *Rode et al*., 2010; *Gu et al*., 2012]. Furthermore, linking a catchment model with an aquatic ecosystem model may be an oversimplification for prediction problems in cases where connecting domains via simple unidirectional boundary conditions is not sufficient (Figures 2b and 2c). Such "aquatic landscapes" may include heterogeneous wetland-dominated environments, lake-rich landscapes, coastal river-estuarine systems, river floodplain systems, and river-reservoir networks. For these examples, each landscape element (e.g., hillslopes, riparian zones, rivers, wetlands, lakes, estuary) has a unique balance of physical and biogeochemical processes [*Oldham et al*., 2013], and a characteristic pattern of connectivity with neighboring systems. Connectivity is critical in shaping habitats and patterns of resource flow, and each subsystem within the network experiences variability along the "isolation-connectivity continuum" [*Leibowitz*, 2003]. In the examples given in Figures 2b and 2c, the regularity of hydrological pulses (either surface or groundwater) determines the degree of isolation or connection with implications of biogeochemistry and ecology. Simulating these environments creates a prediction problem that increasingly demands integration of model types to capture landscape heterogeneity and the complex boundary conditions between the subsystems. Synchrony (or asynchrony) in connectivity regimes of water

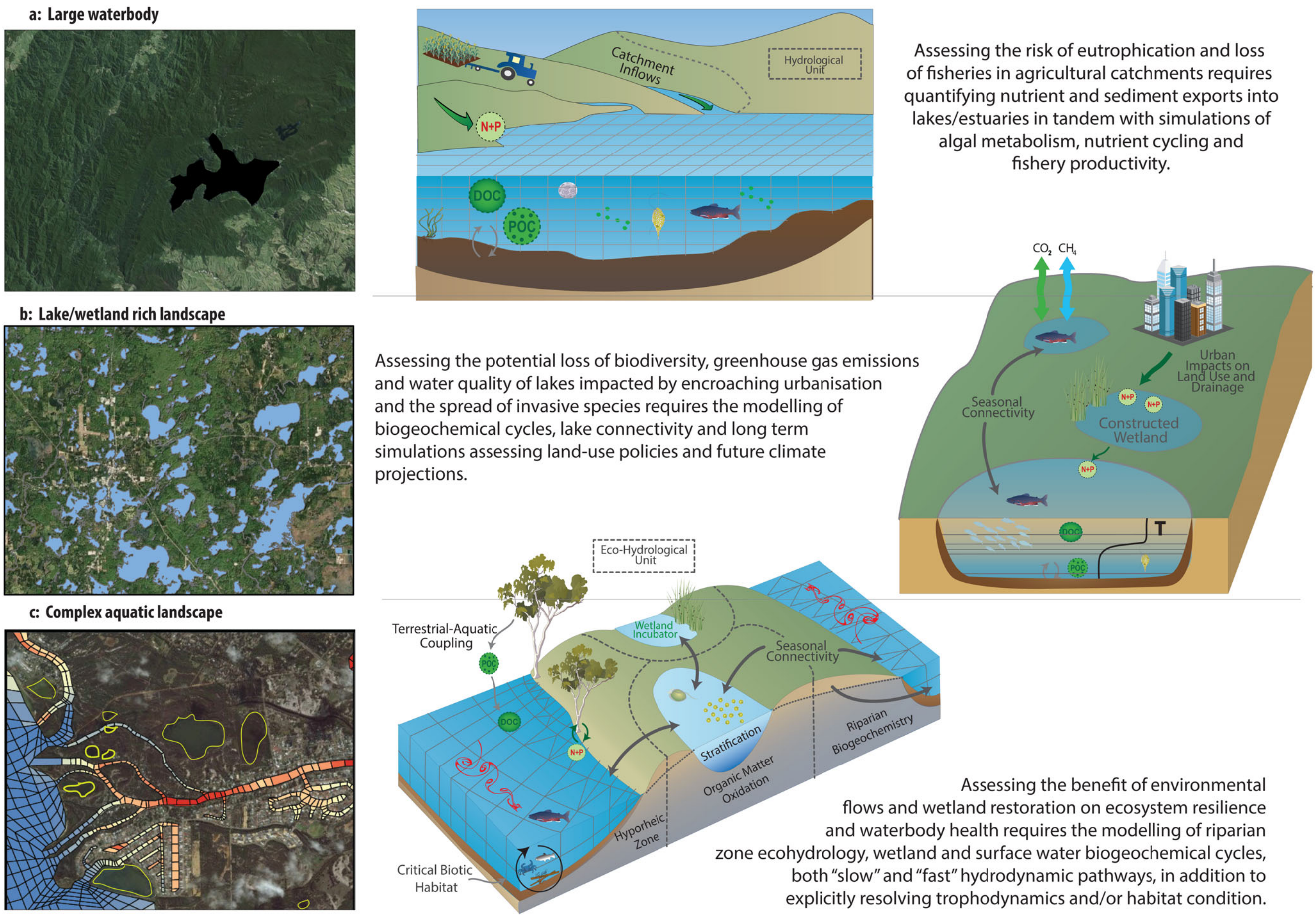

Figure 2. Distinct modeling approaches and model combinations are necessary to holistically assess different landscapes, systems and management or research questions. Examples here show three contexts: (a) a catchment discharging into a large waterbody, (b) a lake/wetland rich landscape, and (c) a complex aquatic landscape.

and material fluxes between the various subsystems is important [*Hernandez and Mitsch*, 2006; *McCluney et al*., 2014], since discrete or seasonal pulses that connect systems can regulate the biotic communities and their interrelationships. For example, within the context of Figure 2c, *Furst et al*., [2014] highlight the "incubation" effect of periodically disconnected floodplain wetlands, whereby zooplankton biomass accumulates before being delivered to the main river food-web when a critical water level thresholds is met, highlighting the importance of designing environmental flow regimes to optimize connectivity of the wetlands.

Our model approaches for simulating the latter examples above are currently inadequate and modular model frameworks able to accommodate simulations in complex aquatic landscapes are essential for scaling up from individual systems to catchments. Whilst progress has been made in simulating at landscape scale across wetlands [e.g., see *Golden et al*., 2014], flexible approaches are required able to support bidirectional linkages of groundwater and surface water subsystems. Such flexible tools would enable managers to compute the multiple services provided within each subsystem and plan intervention in the system more effectively [*Bracken et al*., 2013].

3. Simulating System Resilience, Degradation, and Recovery: How Can Models Meet This Challenge?

Whether focusing on an individual aquatic system or a complex aquatic landscape, finding sustainable management solutions ultimately requires predictions to assess how combinations of stressors impact delivery of ecosystem services over the long-term. The theory of how complex ecosystems respond to stressors has advanced considerably in the past two decades [e.g., *Scheffer et al*., 2012], and efforts are ongoing to explore these dynamics in real-world landscapes [*Carpenter et al*., 2001; *Suding and Hobbs*, 2009; *Peterson et al*., 2012]. The concept of system resilience is built on the idea that positive and negative feedbacks can drive threshold behavior or promote stability in systems in response to stressors, potentially with the emergence of alternative stable states [*Suding et al*., 2004; *Rockström et al*., 2014]. In aquatic systems, it is well established that nutrient loading leads to eutrophication and deterioration in water quality, with the emergence of degraded states that are resistant to recovery [*Smith*, 2003]. However, depending on the context, response pathways may not always follow simple trajectories. Nutrient enrichment may improve some aquatic system attributes (e.g., fisheries) until thresholds are reached, after which it is common to see a switch to dominance of cyanobacteria and an overall deterioration in water quality [*Gal et al*., 2009], and the potential for toxin production and loss of biota. Some cyanobacteria have strong nutrient luxury uptake capacity, thereby amplifying feedbacks of populations with eutrophication [*Cottingham et al*., 2015]. The complexity of nutrient flux pathways within the ecosystem trophic structure can influence this trajectory [*Brookes et al*., 2005]. Once a system is degraded, the various attributes of the system may respond differently to restoration efforts and have different levels of hysteresis, for example, recovery in physicochemical attributes of water quality may not necessarily correspond with the recovery of biotic diversity [*Wildsmith et al*., 2009; *Borja et al*., 2010].

Whether we expect to see a system undergo a gradual transition or one dominated by strong feedbacks and thresholds in response to external pressures (e.g., degradation or rehabilitation) is therefore site and context specific. Process-based models can help in defining and characterizing system behavior, but the ability of aquatic ecosystem models to capture emergent behaviors remains poorly explored. Models of shallow lake ecosystems, however, have been reported to successfully capture alternate stable states (clear, macrophyte-dominated state versus turbid, phytoplankton-dominated state) and hysteresis in response to nutrient loading changes [*Janse et al*., 2010; *Nielsen et al*., 2014]. Furthermore, shifts in dominance of phytoplankton communities to cyanobacteria, indicative of transitional states, have also been simulated [*Elliott*, 2010].

To identify ecosystem tipping points, symptomatic of regime shifts requires multiple stressors to be simulated. Understanding the interactions of nutrient load changes to water bodies in tandem with the effects of climate change is of increasing interest [*Brookes and Carey*, 2011; *Moss*, 2011; *Rigosi et al*., 2015], with several lake model applications addressing this to date [*Nielsen et al*., 2014]. Assessing more complex scenarios that combine pressures from nutrient loading, altered hydrology, warming climate, and shifts in fishing pressure or invasive species are still in their infancy. In most cases these stressors are nonstationary and individually vary over different time scales, creating complex trajectories of ecosystem health (Figure 3). The stochastic nature of the external stressors can also be significant in shaping ecological thresholds. Extreme events in particular, such as pulses of turbid flood waters [*Chung et al*., 2009] or water level decline [*Hipsey et al*., 2014], create transient shifts in function and habitat quality that may drive long-term shifts in ecosystem state. System trajectories will therefore be highly site specific, and there is opportunity for model systems to extend conceptual ideas about resilience and system thresholds by quantifying more fully the evolution of ecosystem state over time for a range of "real-world" systems. With increased ability to predict an acceptable stress range (Figure 3c), a more holistic combination of management actions can be defined. For example, using this approach *Gilboa et al*., [2014] recently defined a composite water quality index as a measure of ecosystem health of Lake Kinneret, and identified a safe operating range in response to nutrient loading and water extraction stressors.

Assessment approaches are required to build confidence that models are able to resolve complex system trajectories. Modelers have traditionally tended to rely on testing model performance at a single point where observations are made. This level of validation is not a robust test of the system-scale emergent dynamics, including resilience, thresholds, and state-shifts, described here as "emergent uncertainty." New procedures and good empirical data sets are required to test the ability of models to capture emergent uncertainty, for example:

1. Emergent dynamics in food-web structure and trophic partitioning;
2. Response to stressors and early warning signals such as critical slowing down, ecosystem flickering, threshold behavior [*Kéfi et al*., 2014];
3. Time lags in response to management changes;
4. Hysteresis during recovery;

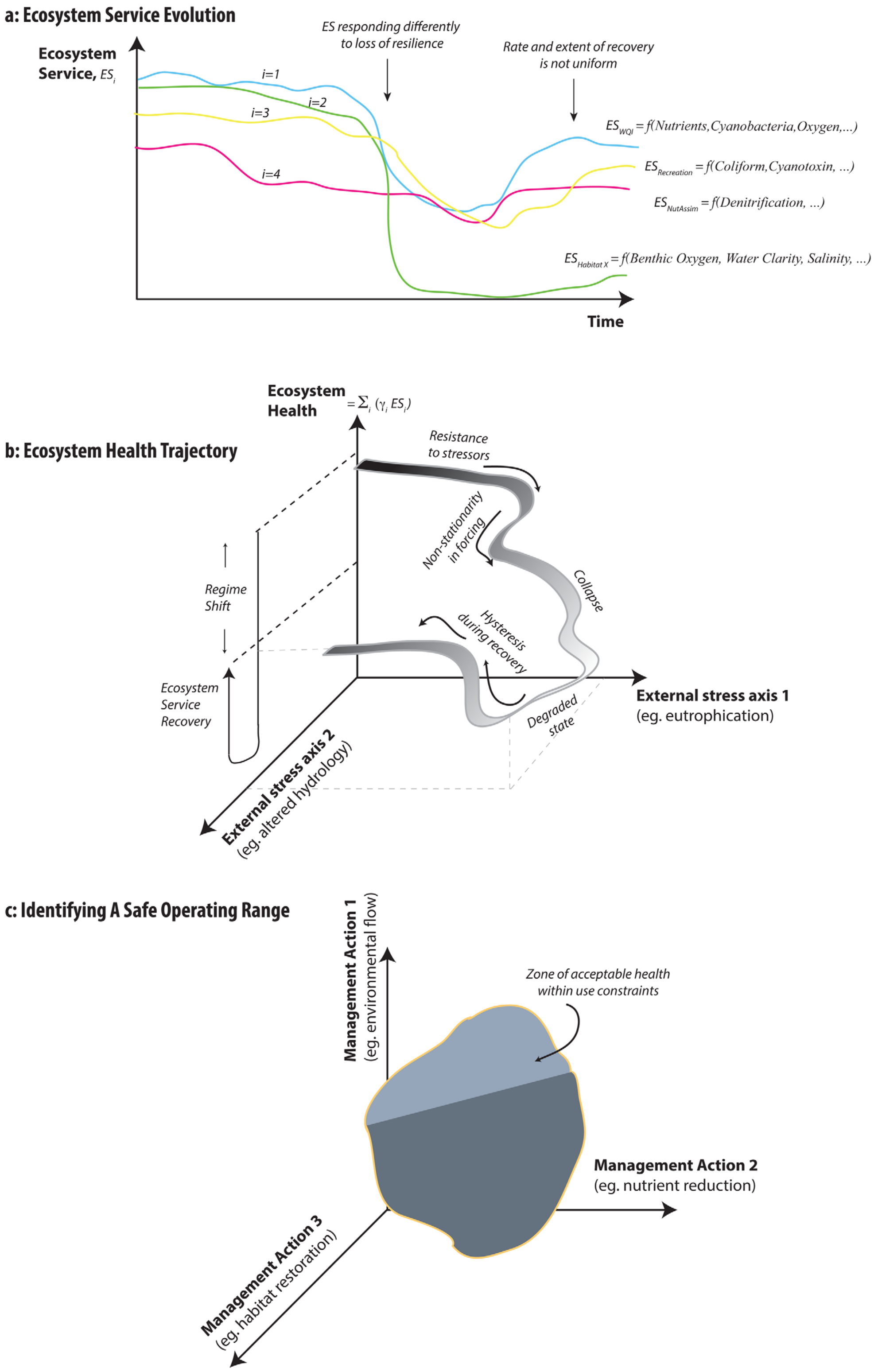

Figure 3. Predicting the evolution of ecosystem health. (a) Historical evolution of hypothetical ecosystem services, ES (WQI = Water Quality Index; Rec = area suitable for recreation; NutAssmin = nutrient assimilation; HabitatX= habitat area for critical biota) computed as a function of model variables as indicated. (b) This generates a complex trajectory in ecosystem state (as indicated by health, computed from summing the ES metrics). (c) Our models can be used to identify management options that give a safe operating range (the shaded area indicates the region whereby the combination of management actions leads to acceptable health; it is truncated on two faces due to constraints such as cost preventing these from being acceptable).

5. Sensitivity of system trajectory to antecedent conditions.

It is unlikely that models can adequately capture all of these system attributes, since abrupt transitions in state are notoriously difficult to predict [*Batt et al*., 2013].

The challenges for model validation described above become more complex at the scale of interconnected landscapes (refer to section 2.3 for context). How the resilience of systems "scales up" remains a topical area for further research [*Hilt et al*., 2011; *Soranno et al*., 2014] and an area where model frameworks that are capable over a range scales can help support advancing our knowledge base. The resilience of a system not only depends upon the interactions of individual components within an ecosystem, but also upon the relationships between connected subsystems [*Hughes et al*., 2013; *McCluney et al*., 2014]. Subsystems can amplify or dampen signals that they are forced by. Humans have extensively impacted patterns of hydrological connectivity through engineering and land cover changes [*Nilsson et al*., 2005; *Kuiper et al*., 2014]. Therefore recovery of these landscapes requires integrated management supported by model frameworks able to capture how connectivity regimes regulate pathways of material flow and impact upon resilience at the macroscale [e.g., *Hilt et al*., 2011].

Prolonged periods of aquatic ecosystem deterioration drive environmental policy changes related to, for example, water extraction, environmental flows, land management, and pollution. The time scale and extent of this response is highly site and context specific [*Meybeck*, 2002], yet critical for identifying long-term sustainable solutions. The "panarchy" conceptual framework highlights the cyclical nature of the feedback between the natural and human systems, making long-term predictions particularly difficult [e.g., *Gunderson and Holling*, 2002]. Model approaches that can move beyond applying human impacts as a boundary condition, and allow two-way integration with socioeconomic and land management models, will ultimately improve links with the needs of policy makers and will inevitably demand simulations over long-time periods [*Elshafei et al*., 2014], and compound issues of predictive uncertainty. This has challenged the hydrological community to comprehensively consider the link between data, models, and predictions in the quest for improved understanding of how catchments vary under changing conditions [*Ehret et al*., 2014]. The prospect of models able to learn from new data streams offers the potential for predictive ability to be continually updated and uncertainty progressively reduced, even as unexpected events occur [*Thompson et al*., 2013]. Developing a mechanism whereby this can be achieved within observatory systems therefore offers an attractive approach to organize information in a way that better enables scientists and decision-makers to tackle this long-term prediction problem.

4. Learning From Data: Observatories as a Knowledge Integrator

The hydrological community is increasingly undertaking real-time observations and predictions of systems with the ambition to provide forecasts at scales from days to decades [*Liu et al*., 2012; *Mackay et al*., 2015]. The development of integrated environmental observatories that combine data from distributed sensing systems and model infrastructure offers benefits in terms of automating aspects of model operation (e.g., model integration and automatic calibration) [*Werner et al*., 2013]. Within the context of aquatic systems, approaches to address the prediction challenges outlined in the previous sections through integration of models within observatories systems has yet to be fully explored. Within this section it is our aim to outline a framework for the evolution of predictive skill, whereby observations from sensing infrastructure and traditional monitoring are integrated with flexible model libraries that may be used to create a diverse range of custom model structures. The framework has been designed to demonstrate a potential pathway for integration of bottom-up (process-based) and top-down (data-driven) approaches within an adaptive loop and guided by theoretical insights (Figure 4). In this section, we expand on key aspects of the framework to explore how observatory systems can fundamentally advance our understanding of how aquatic systems respond to change, whilst also discussing how outputs can be more effectively communicated to stakeholders.

4.1. Sensor Networks for Aquatic Systems

There has been a major proliferation of sensors relevant to measurements of hydrological, water quality, and aquatic habitat properties. Real-time sensor deployments for measuring water quality properties (e.g., dissolved oxygen, chlorophyll-a, and turbidity) from multiparameter sondes are now routine, and sensors

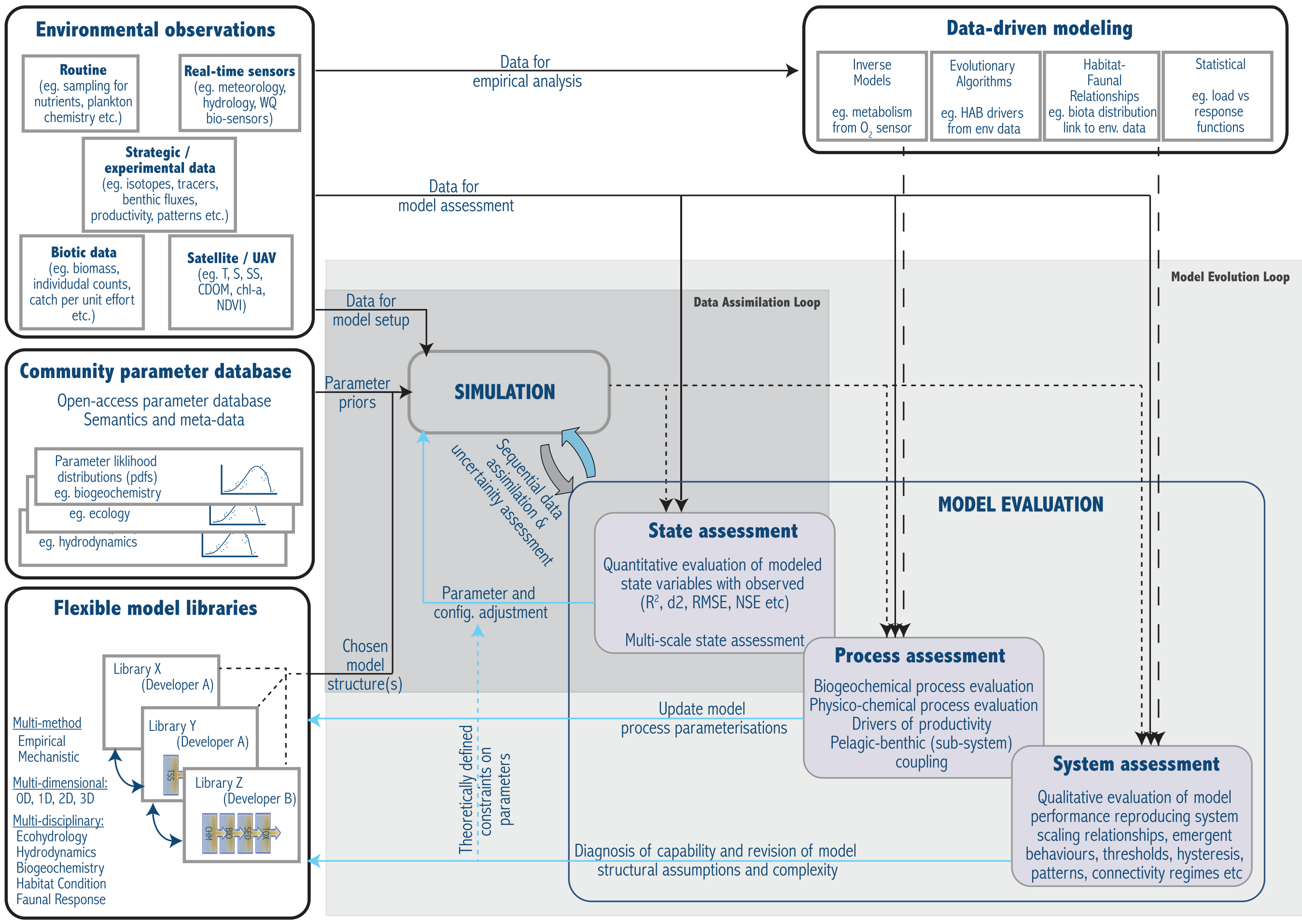

Figure 4. Schematic overview of model learning from diverse data streams. Two learning cycles are identified: the short-term data assimilation loop (dark grey) and the long-term model evolution loop (light grey). Model evaluation practices are categorized as assessing model state, process, or system-level predictions. The latter two comparisons seek to match the process-based model function with empirically derived patterns, either from direct observations (solid black line) or via interpretation from data-driven models (large dash line).

can also measure variables such as dissolved organic carbon (DOC), phycocyanin, and nitrate [*Neal et al.*, 2012; *Wild-Allen and Rayner*, 2014]. The next decade holds great promise for new in situ measurement technologies. For example, advanced measurements such as stable isotope measurements [*Herbstritt et al.*, 2012], heavy metals [*Warnken et al.*, 2009], and biosensors [*Shade et al.*, 2009] are transforming our ability to monitor aquatic systems. Biotechnological advances are also opening up opportunities for real-time PCR and microbial measurements, for example of pathogens [*Ikonen et al.*, 2013; *Lopez-Roldan et al.*, 2013], and online monitoring of phytoplankton diversity using flow cytometry [*Pomati et al.*, 2013]. While sensors that measure some fundamentally important aquatic attributes have yet to be developed or are currently prohibitively expensive for widespread use (e.g., sensors for methane or phosphorus), this field is rapidly advancing and has great potential for developing observational data sets that can be used to calibrate and validate ecosystem models.

To complement the high temporal resolution data streams, satellite products for synoptic surveys of water quality in wetlands, large rivers, estuaries, and lakes are also creating new opportunities for understanding controls on ecosystem attributes [*Palmer et al.*, 2015]. Data products derived from satellite observations can yield spatially resolved water quality indices [*Kloiber et al.*, 2002; *Moore et al.*, 2014; *Allan et al.*, 2015] in addition to changes in water quantity [*Prigent et al.*, 2012], and generate long-term "virtual" time series [*Schneider and Hook*, 2010]. These data sets create new scope for validating models across multiple spatial scales.

Data collected through citizen science initiatives is becoming increasingly important for environmental monitoring purposes due to the increasing emphasis on understanding the intertwining dynamics of humans with the environment. For example, advances in mobile devices can complement primary data streams (those identified in Figure 4), and are particularly useful for capturing data for which sensors are not available, e.g., bird counts and fish catch per unit effort [*Dickinson et al*., 2012; *Lottig et al*., 2014; *Thorson et al*., 2014]. Additionally, the use of unstructured data, for example, qualitative data on catchment use and public perception of environmental condition derived from automatic web searching, can be integrated with traditional data streams. These data streams may not be appropriate for supporting direct evaluation of models, but offer potential to help prioritize concerns of community stakeholders and identify user demand for scenario assessments.

4.2. Model Evolution Within Observing Systems

The diversity and density of data from sensor networks, in conjunction with data from conventional assessments, requires advanced tools and workflows to convert the data into information. Seamless integration of the data with process-based models can be used to improve model setup (e.g., better boundary conditions), and model calibration. Since many process-based models tend to be overparameterized [*Arhonditsis et al*., 2008], more diverse and high-resolution observations create advantages for testing the rigor of models at scales relevant to the dominant underlying processes [e.g., *Kara et al*., 2012; *Hamilton et al*., 2014; *Bruesewitz et al*., 2015].

The search for more formal approaches to reduce model error through better integration with empirical data has been the topic of significant analysis, particularly within the hydrological community [e.g., *Gupta et al*., 2012; *Parrish et al*., 2012; *Thompson et al*., 2013; *Robson*, 2014b]. Optimization of parameters and assessing uncertainty in short to near-term forecasts has been made possible through application of Bayesian Hierarchical Frameworks (BHFs) in aquatic ecosystem models [*Zhang and Arhonditsis*, 2009; *Dietzel and Reichert*, 2014]. Running models within an observatory context allows this to be undertaken as part of a sequential data assimilation procedure, using techniques such as the Ensemble Kalman Filter (EnKF) algorithm [*Kim et al*., 2014b], and in some cases enabling continual (time-varying) updates to parameter posteriors. Such data assimilation techniques, however, have had limited application for water quality assessments (relative to hydrological applications), and in particular for multidimensional aquatic ecosystem models of lakes, large rivers, and estuarine environments [*Robson*, 2014b]. This is thought to be due to the difficulty and expense of collecting adequate water quality and ecosystem data sets to support application of data assimilation algorithms, and the excessive computational demands when many interacting variables are being simulated. Some techniques have emerged whereby modelers undertake an optimization of parameters on a spatially reduced form of a biogeochemical model prior to a high-resolution simulation as a practical solution [*McDonald et al*., 2012] (Adiyanti et al., Stable isotopes reduce parameter uncertainty of an estuarine carbon cycling model, *Environmental Modelling and Software*, in review). However, improvements in distributed computing are opening up opportunities for data assimilation of 3-D models, as recently exemplified in the ocean modeling community [*Xiao and Friedrichs*, 2014].

Whilst advances in the resolution and diversity of data sets within observatory systems will likely drive rapid advances in data assimilation tools, there are limits to how far data assimilation alone could improve predictions, particularly given the nature of the simulations required for integrated assessment. Model structural inadequacy leads to error that is unresolvable but identifiable [*Gupta et al*., 2012], and once identified can be used to support model updates. Specifically, *Thompson et al*. [2013] summarized four ways that model-data learning can support predictions in systems subject to non-stationary (and potentially unexpected) drivers: (i) by reducing uncertainty in short to near-term forecasts; (ii) by identifying model weaknesses in reproducing essential system-level dynamics, and updating model structures or approaches as the system of interest undergoes change; (iii) by identifying deviations from expected system behavior which may be attributable to previously undetected feedback mechanisms; and (iv) where "hotspots" are noted, adapting monitoring programs to better inform predictions, thus optimizing investment in environmental monitoring. With this in mind, the approach outlined in Figure 4 identifies that model operation must be embedded within a learning framework that supports adaptation of model parameters, structure and function, and this is divided over two separate (but potentially interacting) loops: the data assimilation loop and the model evolution loop.

Within the model evolution loop, the focus is on diagnostic evaluation of the models ability to reproduce theoretically relevant metrics of aquatic system behavior. In Figure 4, several examples are categorized into signatures related to physical or biogeochemical process rates, and system-scale emergent properties relevant to the discussion presented in section 3. As has recently been demonstrated within hydrological models [*Vrugt and Sadegh*, 2013; *Shafii and Tolson*, 2015], signatures of system function may in fact serve to constrain the model calibration. Moreover, as experience is gained in identifying model shortcomings, the question then becomes—can we dynamically adapt model structure to learn from new trends and patterns present in the observational data?. This could be achieved through assessment of model ensembles or changes to model functionality over time. There is a largely unexplored role here for data-driven models to help shape predictions in concert with process-based models. As identified in the top right of Figure 4, empirical relationships that may not have been anticipated or fully explored during model design (e.g., those outlined in section 3), may then be used to guide updates, refinements, or replacement of model components within the libraries on which the model simulation was built.

On a practical level, there are therefore several ways updates to models and predictive ability can occur:

1. Data assimilation: sequential updating of model parameter likelihood distributions as new information derived from a sensor network is available and processed. Besides improved parameter estimates, an outcome is the potential to develop reanalysis products that provide a temporally continuous and spatially explicit estimate of the true state of the system based on assessment of observations and models.
2. Augmenting simulations by mechanistic models with data-driven models: The quality of mechanistic model simulations is often heavily impacted by poorly resolved boundary condition specification, particularly since essential biogeochemical and ecological variables are infrequently measured in input tributaries to many systems. Use of data-driven tools to develop models for boundary condition concentrations offers the potential to reduce input error in this regard. Alternatively, use of machine-learning methods can be used to predict the error structure of mechanistic model simulation output, and the joint prediction reported to stakeholders (not shown in Figure 4).
3. Use of model-structure ensembles: approaches such as Bayesian Model Averaging (BMA) have been introduced to identify the best model approaches for a given data set [*Ramin et al*., 2012]. When employed to assess competing model structures, there is potential for this approach to define adequate levels of complexity for any given system under changing conditions [*Parrish et al*., 2012].
4. Dynamic algorithm reparameterization: In this case, sufficiently flexible model packages that contain libraries of alternate algorithms for specific processes (e.g., the photosynthesis-irradiance relationship), would be sampled to identify the best combinations to match observations [*Recknagel et al*., 2008a; *Ramin and Arhonditsis*, 2013]. Potential exists here for direct interpretation of sensor data using data-driven model approaches. For example, computation of ecosystem metabolism from raw oxygen sensor data [*Hanson et al*., 2008] may subsequently be applied to constrain metabolism predictions within the model simulation by applying justified constraints on parameter space (as indicated in Figure 4), or reparameterizing the relevant expression within the model library.
5. Adaptive configuration of model structure: on occasion, field measurements will reveal behavior that is not predicted by the models because the process or variable has not yet been configured appropriately within the chosen model algorithms. Assessment of new observations, such as the emergence of unexpected phytoplankton species, can be used to update model configuration. Furthermore, application of "black-box" models, such as artificial neural networks or similar, to the observatory data may identify controlling environmental factors [*Coad et al*., 2014], that were not obvious a priori but could inform subsequent changes to model configuration.
6. Dynamic updates to model resolution: where it is assessed that model predictions are inadequately capturing temporal or spatial variability in ecosystem attributes, increasing model dimensionality, or refining model resolution can be undertaken, for example, through automated nesting or regridding of models. Furthermore, assessing the relative performance of models of different scale can be seen as a mechanism to identify the limits of predictability of any chosen model, thereby guiding modelers through challenges raised in section 2.

Although these mechanisms are suggested in general terms, the intention is to highlight future opportunities for model-learning frameworks to support the hybridizing of process-based and data-driven models. This is only achievable with flexible model systems where modelers are able to easily design and test models of different resolution, complexity, and philosophy, both through quantitative and qualitative means. Whilst many technical challenges remain to realize such a framework, the process of model evolution over time presents not only an opportunity to improve predictions, but also an opportunity to facilitate the engagement of stakeholders, allowing them to build confidence in the suitability of various model approaches.

4.3. Quantifying and Communicating Ecosystem Condition and Service Delivery

The ongoing interaction of models with observations can allow us to capture the systematic feedbacks between observation, prediction, and management that emerge under continuously changing conditions [*Clark et al*., 2001; *Reed et al*., 2006]. However, often the best scientific knowledge is not translated into policy. In the context of online observatory systems, rich data streams and more accurate model predictions can be supplied to stakeholders, but there is evidence to suggest that simply supplying information from data or models is unlikely to lead to positive environmental outcomes [e.g., *Hart and Calhoun*, 2010]. The problem of many emerging observatory systems that communicate data is that the information provided is not readily digestible by those needing to make the decisions. More complex integrated models of hydrology, hydrodynamics, biogeochemistry, ecology and society, and novel data streams only amplify this problem. An approach to successfully disseminate insights from the models and data streams is to not rely on raw data from sensors or simulation output when communicating system properties, but focusing on user demands and their requirements for information [*Mackay et al*., 2015]. The question then becomes, what critical information do we need to distill from the sensors and models (or reanalysis products) to facilitate the ongoing engagement of decision-makers and catchment communities in the process? For example, to communicate that a system is experiencing regular hypoxia it may be more effective to present the relative reduction in suitable habitat for benthic biota rather than time series of dissolved oxygen. Since modeled variables may not necessarily be easily translated directly into metrics used by ecologists or decision makers, dedicated efforts are required to identify proxies, such as for ecosystem service provision and resilience [*Carpenter et al*., 2001].

Collectively, a suite metrics that are tailored to local systems can serve as indicators of ecosystem health, offering an improved way to communicate data from an observatory to managers and the public (Figure 5). This process has the potential to add value to agency or ad hoc monitoring initiatives since, through the observatory system, it would allow immediate translation of new monitoring data into attributes of direct relevance to stakeholders. By adopting Bayesian schemes outlined in the previous section, then the value of new observations on improving model accuracy is quantifiable, and the updated models become available to undertake an improved assessment of health metrics and forecasts of future trajectories. Ideally, this would ultimately strengthen connections between knowledge and action [*Hart and Calhoun*, 2010], with direct translation to information for policymakers [*Soranno et al*., 2015]. A well-designed information portal delivering essential information would promote effective dialog and empower communities to more actively participate in understanding their local catchment, and provide a vehicle for adding value to citizen science data-collection initiatives.

5. Enabling a Community-Driven Assessment of Complex Aquatic Landscapes

To realize the technical advances outlined above requires a high level of interdisciplinarity and flexibility in software development, requiring participation from domain experts, informaticists, software developers, and information brokers. A theme in recent transformative science expeditions (e.g., Large Hadron Collider; genome sequencing project) is an engaged group of diverse collaborators from multiple institutions. High-performing research teams that emerge within effective networks create research outcomes that are more than the sum of the parts [*Cheruvelil et al*., 2014]. Within the environmental sciences, research communities have begun to generate momentum from the "open data" trend, especially with the creation of open source tools and model frameworks [*Trolle et al*., 2012]. We further advocate for a research structure that includes open sharing of all elements of the scientific process (ideas, models, tools, and data) as being essential to link theoretical developments and model infrastructure.

5.1. Innovating Aquatic System Assessment Through Open Communities

The emergence of "network science" as a vehicle to advance software and synthesis efforts is critical for setting the agenda and driving transdisciplinary collaborations. Science communities that embody openness have enabled researchers to tackle larger, more complex problems, despite some degree of resistance to data sharing [*Soranno et al*., 2015]. Synthesis activities within communities are critical to identify "universal"

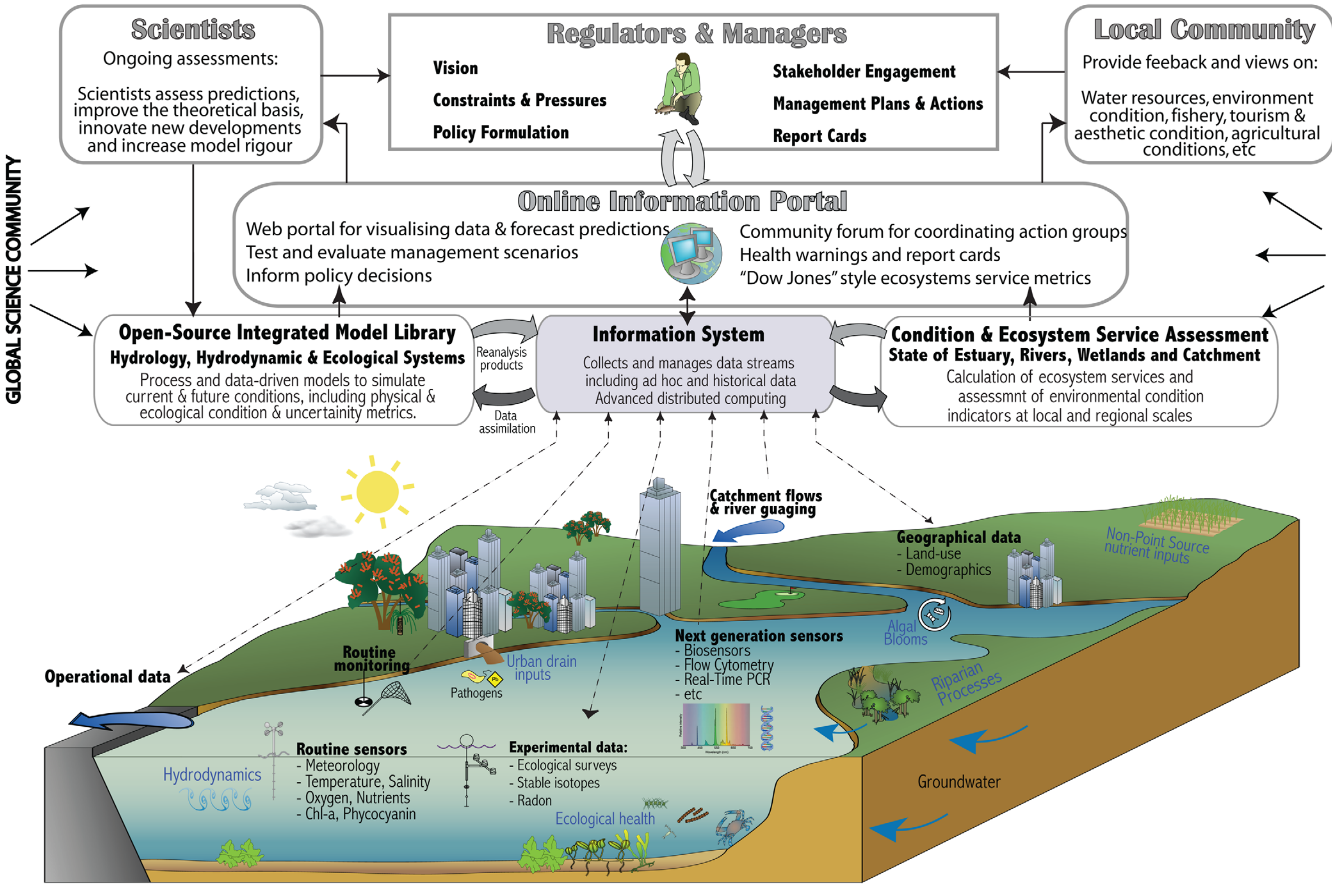

Figure 5. Overview of an aquatic system observatory showing the interrelationships between observations, predictions, and management.

descriptors of processes, similarity in emergent behaviors, and how water quality, nutrient, and contaminant pathways vary across geomorphologic and climate gradients [*Blöschl*, 2006; *Sivapalan et al.*, 2011]. Whilst synthesis efforts have historically been undertaken separately in the hydrological and ecological disciplines, there is a need for synthesis of the ideas and data in the context of the technological needs and model frameworks identified in section 4. Specifically, the collation and sharing of site-specific process-data spanning environmental gradients can facilitate the development of an improved evidence base for guiding the choice of model resolution and process complexity, helping us address the challenges of section 2 through the diagnostic evaluation step depicted in Figure 4. Importantly, large gradients of ecosystems provide a diversity of data for confronting models and defining the range over which they are suitable. Synthesis activities can also encompass systematic model comparisons, whereby model structures and integration of different methods can be better scrutinized [*Schmolke et al.*, 2010]. Activities such as model intercomparison projects (MIPs) and ensemble model predictions can identify model approaches that are most suited to particular application contexts [*Trolle et al.*, 2014].

A specific example, that motivated the development of the framework in Figure 4, is the grass-roots Global Lake Ecological Observatory Network (GLEON), whose scientists collect and share real-time sensor data from a variety of lacustrine environments from around the world [*Hanson*, 2007; *Hamilton et al.*, 2014]. Other networks such as the Consortium of Universities for the Advancement of Hydrologic Science, Inc. (CUAHSI), and the Critical Zone Observatory (CZO), have similarly fostered the community-driven development of software infrastructure, collation of diverse data sets and science workshops. Network science provides an opportunity for all to participate provided there is a common ethos of cooperation, collaboration, and trust. The curated large-scale data sets within these networks have unquestioned research value [*Vogel et al.*, 2015]. By individuals and organizations committing to providing data openly, researchers can (a) see their data more thoroughly interrogated and (b) contribute to regionalization and synthesis efforts. Within the hydrological sciences, this approach has been established through initiatives such as the international Model Parameter Estimation Experiment [MOPEX, *Duan et al*., 2006] and synthesis activities where the power of comparative analysis has been demonstrated [e.g., *Blöschl et al*., 2013]. Examples are emerging of the application of GLEON data to conduct comparative studies relevant to the challenges identified in this paper [*Klug et al*., 2012; *Read et al*., 2012; *Solomon et al*., 2013], but these can be better facilitated through standards defining water quality attributes (particularly beyond physicochemical properties) and efforts to create data products. Ultimately, products developed within these communities must meet their diverse needs of modelers by striking a balance between supporting standardization versus innovation.

5.2. Shared Libraries of Models, Tools, and Parameter Values

There are many open source codes that are now used for water quality and aquatic ecosystem prediction (e.g., HYPE, SWAT, PIHM, QUAL-2K, MODFLOW, FABM, DATM, DELFT3D, MOHID, AED etc.). Open source code exposes model algorithms, encourages trust, and provides inspiration for the next generation of models. There is a general view that active communities collaborating on code development and sharing experiences speed up the development and testing process by involving more people and not reinventing established algorithms [*Mooij et al*., 2010], and the transparency of code provides a mechanism for quality assurance and facilitates review of scientific work. Beyond simply being more efficient, many of the questions being asked of models are highly complex, and developments require a large and diverse group of collaborators from multiple institutions. Open source code development and online version management now routinely support multiple remote contributors and provide accounting for attribution.

In order to accommodate a diversity of applications, research questions, and address issues of model complexity identified in section 2, the proposed framework further advocates for the creation of libraries of flexible model objects [e.g., *Trolle et al*., 2012; *Bruggeman and Bolding*, 2014; *Mooij et al*., 2014], that can work with model-learning workflows. The objects might include a spectrum of modules from microbial function to physical processes, allowing users to experiment with model structure, rather simply "rolling out" standard model configurations. Such libraries can archive alternate algorithms for empirically observed processes across a diversity of sites within science networks, thereby underpinning model adaptation approaches [*Recknagel et al*., 2008b]. In parallel to flexibility in process configurations, spatial dimensionality and system compartmentalization will increasingly be simulated via a diverse array of physical drivers (e.g., hillslope model, wetland/floodplain model, river model, lake model, estuary model) that need to link to biogeochemical and ecological reaction libraries, and this requires standards and a common vocabulary within such a collection.

To accelerate the ability of the model development community to develop learning frameworks, as outlined in Figure 4, an overarching blueprint is required that can link diverse model libraries, data assimilation frameworks, and model automation in a manner that can accommodate the diversity of model form. The need for state updating in particular requires a high level of interaction with models that can be difficult to retrofit into legacy codes. Furthermore, there is a need for common model typologies and interfaces, shared semantics, and flexible analytical frameworks, with general progress in this area advanced by initiatives such as OpenMI. New workflows for integrating software frameworks for data assimilation within observatory systems are also recently emerging. For aquatic ecosystem prediction, further advances require investment in the development of community-endorsed parameter libraries, allowing modelers to easily gain access to parameter prior distributions for model uncertainty assessment. Finally, approaches to guide the development of community-endorsed reanalysis products are required, since this has received limited attention in the context of aquatic ecosystem prediction, yet have the potential to provide the best quality information to researchers and decision-makers.

Underpinning our desire for sharing model code is the ability of modelers to accurately report on and assess model performance. Decisions about validation, however, have historically been largely ad hoc and past meta-analyses on aquatic biogeochemical models accuracy have highlighted that prediction skill has barely advanced over the past several decades [*Arhonditsis et al*., 2006; *Robson*, 2014a]. This highlights the need for agreement on improved assessment approaches as a means to better identify when a model is appropriate for its intended use. Standards in reporting can serve to increase reproducibility and predictive capabilities [*Jakeman et al*., 2006; *Robson et al*., 2008], and as we seek to assess alternate model approaches against a larger number of data streams there is a need to devise general strategies to report on model predictions.

As in other environmental modeling communities, widely agreed upon assessment protocols for model performance that encourage a more rigorous validation of models will serve to create standards and a common vocabulary that will ultimately support comparisons and synthesis between model applications [*Harmel et al*., 2014]. As identified in section 4.2 and the "model evolution loop" in Figure 4, extending assessment to also include metrics and characteristic signatures relevant to ecosystem function is critical, and moving beyond typically computed error statistics remains an area that requires consensus on the approaches that are most appropriate for different motivating questions and levels of model complexity.

6. Conclusions

In the face of increasing anthropogenic stressors, scientists can use aquatic ecosystem models to identify sustainable solutions for managing water resources. Despite the diversity of models available, in many contexts it remains difficult to holistically assess the impacts of multiple stressors and/or the benefits of management interventions. Historically, the focus has been on developing models for exploring nutrient cycling, eutrophication processes, and other drivers of water quality degradation. Whilst great advances have been made in broadening the scope of simulations, expanding process complexity and developing integrated model packages to support management needs, we have identified areas where advances in models are required to provide more holistic predictions. Furthermore, except for a few examples, it is unclear how well they capture system-level properties such as resilience and other emergent behaviors, yet it is essential we have confidence in the ability of models to reproduce these features if they are to be used to plan rehabilitation and restoration, and support assessments of how climate change will impact upon systems.

The expanding repositories of data now being collected through distributed sensor networks, in addition to advances in model assessment and calibration approaches, has created new opportunities for how we can undertake prediction. An essential aim of the paper has been to bring together ideas from both the hydrological and ecological literature and present a framework for model learning within observatory systems that pays attention to the varied motivations for modeling whilst also being cognizant of technical limitations. An essential component of the framework is the development of flexible model libraries, rather than the adoption of a single model of choice. Carefully constructed model libraries can allow us to identify levels of process complexity and scale that are adequate to capture trends in observations. They also offer potential for data-driven algorithms or models to be integrated with process-based simulations, thereby bridging bottom-up and top-down lines of enquiry. The scale and transdisciplinary nature of the prediction challenge requires extensive collaboration and we therefore outline network science initiatives as a means to (a) lead to the develop of community-driven open-source software and application workflows, and (b) undertake synthesis activities and develop consensus on theoretical metrics that may be used to guide model assessment and adaptation.

Improved prediction will help us both explore theory and support decision-making. However, in order for them to support shifts in policy and communicate system health, we need to generate meaningful metrics of system health, and communicate the level of uncertainty in our predictions. Further effort is required to identify model proxies that can be used to summarize how ecosystem service provision varies in response to anthropogenic change. Ultimately, integrating model predictions within observatory systems offers the advantage of increasing the worth of data to management agencies and encourages a tight feedback between observation, understanding, and on-the-ground actions.

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