Progress and opportunities in advancing near-term forecasting of freshwater quality

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Abstract

Near-term freshwater forecasts, defined as sub-daily to decadal future predictions of a freshwater variable with quantified uncertainty, are urgently needed to improve water quality management as freshwater ecosystems exhibit greater variability due to global change. Shifting baselines in freshwater ecosystems due to land use and climate change prevent managers from relying on historical averages for predicting future conditions, necessitating near-term forecasts to mitigate freshwater risks to human health and safety (e.g., flash floods, harmful algal blooms). To assess the current state of freshwater forecasting and identify opportunities for future progress, we synthesized freshwater forecasting papers published in the past five years. We found that freshwater forecasting is currently dominated by near-term forecasts of water quantity and that near-term water quality forecasts are fewer in number and in early stages of development (i.e., non-operational), despite their potential as important preemptive decision support tools. We contend that more freshwater quality forecasts are critically needed, and that near-term water quality forecasting is poised to make substantial advances based on examples of recent progress in forecasting methodology, workflows, and end user engagement. For example, current water quality forecasting systems can predict water temperature, dissolved oxygen, and algal bloom/toxin events five days ahead with reasonable accuracy. Continued progress in freshwater quality forecasting will be greatly accelerated by adapting tools and approaches from freshwater quantity forecasting (e.g., machine learning modeling methods). In addition, future development of effective operational freshwater quality forecasts necessitates substantive engagement of end users throughout the forecast process, funding, and training opportunities. Looking ahead, near-term forecasting provides a hopeful future for freshwater management in the face of increased variability and risk due to global change, and we encourage the freshwater scientific community to incorporate forecasting approaches in water quality research and management.

Progress and opportunities in advancing near-term forecasting of freshwater quality

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Abstract

Near-term freshwater forecasts, defined as sub-daily to decadal future predictions of a freshwater variable with quantified uncertainty, are urgently needed to improve water quality management as freshwater ecosystems exhibit greater variability due to global change. Shifting baselines in freshwater ecosystems due to land use and climate change prevent managers from relying on historical averages for predicting future conditions, necessitating near-term forecasts to mitigate freshwater risks to human health and safety (e.g., flash floods, harmful algal blooms). To assess the current state of freshwater forecasting and identify opportunities for future progress, we synthesized freshwater forecasting papers published in the past five years. We found that freshwater forecasting is currently dominated by near-term forecasts of water *quantity* and that near-term water *quality* forecasts are fewer in number and in early stages of development (i.e., non-operational), despite their potential as important preemptive decision support tools. We contend that more freshwater quality forecasts are critically needed, and that near-term water quality forecasting is poised to make substantial advances based on examples of recent progress in forecasting methodology, workflows, and end user engagement. For example, current water quality forecasting systems can predict water temperature, dissolved oxygen, and algal bloom/toxin events five days ahead with reasonable accuracy. Continued progress in freshwater quality forecasting will be greatly accelerated by adapting tools and approaches from freshwater quantity forecasting (e.g., machine learning modeling methods). In addition, future development of effective operational freshwater quality forecasts necessitates substantive engagement of end users throughout the forecast process, funding, and training opportunities. Looking ahead, near-term forecasting provides a hopeful future for freshwater management in the face of increased

variability and risk due to global change, and we encourage the freshwater scientific community to incorporate forecasting approaches in water quality research and management.

Keywords: Data assimilation, Ecological forecasting, Hydrological forecasting, Hindcast, Near-term iterative forecasting cycle, Uncertainty, Water quality

Introduction

Near-term ecological forecasts, defined here as future predictions of physical, chemical, or biological variables at sub-daily to decadal scales and incorporating uncertainty (Fig. 1; Dietze, 2017), are increasingly being developed to understand and predict the future of ecosystems (Lewis et al., 2022). Forecasts of future ecosystem conditions enable preemptive management, enabling decision-makers to prevent or mitigate risk (e.g., Berthet et al., 2016; Fujisaki-Manome et al., 2022). Among ecosystems, forecasts of freshwater ecosystems (i.e., lakes, rivers, wetlands) may be particularly valuable, as freshwaters have been more negatively impacted by human activities and global change than terrestrial or marine ecosystems (Albert et al., 2021; Moorhouse & Macdonald, 2015), necessitating new approaches for their management.

The acute threats to freshwater ecosystems from global change (Field et al., 2014; Maasri et al., 2022) highlight the potential of near-term freshwater forecasting for advancing water management and freshwater resource use, as well as our understanding of freshwater ecosystems (Bradford et al., 2018, 2020; Coreau et al., 2009). Recent advances in next-generation technology for environmental monitoring of a broad range of freshwater ecosystem variables via *in situ* sensors, satellites, and internet of things (IoT) networks (Hestir et al., 2015; Marcé et al., 2016; Singh & Ahmed, 2021); development of diverse modeling, data assimilation, and uncertainty propagation methods in ecological studies (e.g., Chen et al., 2021; Heilman et al., 2022; Varadharajan et al., 2022); and a growing community of practice around ecological forecasting (Dietze & Lynch, 2019) are synergistically facilitating the increased production of near-term freshwater forecasts (Fig. 2).

These advances present opportunities for freshwater scientists to integrate new tools and skills into forecasting efforts. In this review, we analyze the recent progress of freshwater forecast development, i.e., the variables being forecasted and methods used, the accuracy of recently developed forecasts, and the application of forecasts for different end users. We identify future opportunities for advancing freshwater forecast production and use, and outline recommendations forward for galvanizing the freshwater quality forecasting community.

Motivation for freshwater forecasting

Recent efforts in near-term freshwater forecasting have been motivated in many cases by the increased variability of freshwater ecosystems due to global change (Bradford et al., 2018; Gilarranz et al., 2022; Reggiani et al., 2022). Forecasts are most useful when they provide actionable information about future conditions that was previously unknown: e.g., there is no need for setting up a forecasting system generating month-ahead forecasts if next month's water quality conditions are consistently identical to today's water quality conditions. Unfortunately, the increased ecosystem variability experienced by many freshwaters under global change precludes the use of historical baselines to inform our expectation of their future conditions (Bradford et al., 2018; Gilarranz et al., 2022; Millar & Woolfenden, 1999). Much of this variability is occurring on short time scales (days to seasons) and is manifested across physical, chemical, and biological freshwater variables. For example, intense drought and floods due to climate change are altering water quantity in lakes, rivers, and wetlands (Davenport et al., 2021). Similarly, dissolved oxygen concentrations, a key control on freshwater quality, are declining in temperate lakes worldwide as water temperatures warm (Jane et al., 2021) and peak summertime algal bloom intensity increases (Ho et al., 2019). These examples are a few of the many physical, chemical, and biological changes that are being experienced by freshwater ecosystems worldwide in response to global change.

Near-term forecasting provides critically-needed opportunities for proactive, preemptive management of freshwater ecosystems to conserve and protect ecosystem health and services in response to increased variability under global change (Bradford et al., 2018, 2020; Reggiani et al., 2022). For example, if managers had advance warning of a future flood, they could preemptively re-route traffic from low-lying areas or coordinate evacuations to minimize human risk (Berthet et al., 2016). Similarly, a forecast of potential water quality impairment due to low dissolved oxygen levels or an intense algal bloom could allow managers to preemptively plan reservoir water releases, activate aeration systems (Quinn et al., 2005), or inform recreational beach closures (Choi et al., 2022). As much of the environmental variability currently exhibited in freshwater ecosystems is expected to intensify in the future under global change, it is critical to develop freshwater forecasts now.

Overview of the near-term, iterative forecasting cycle

Many near-term forecasting systems use the iterative forecasting cycle as their foundation (Fig. 1; Dietze, 2017), which includes: engagement of end users; coordination of the forecasting team; model, infrastructure, and workflow development; data collection; uncertainty quantification; data assimilation (Table 1); forecast generation; forecast assessment; and dissemination to end users. Ideally, targeted freshwater forecast end users (e.g., managers, natural resource decision-makers) are engaged at the beginning of the forecast process to identify: 1) first, whether a forecast would assist in achieving end user goals; 2) if yes, then which forecasted variables are needed; and 3) the frequency and method of forecast dissemination (e.g., Berthet et al., 2016; Fujisaki-Manome et al., 2022; Gerst et al., 2020; Fig. 1 Step A). If end users have determined a freshwater forecast is needed, a forecasting team must be assembled and coordinated, likely including members with expertise in freshwater science, freshwater modeling, data collection (e.g., sensors, remote sensing), cyberinfrastructure, water management, and end user engagement (Carey et al., 2022; Fig. 1 Step B). The team will then work to develop the models, infrastructure, and workflows needed to produce forecasts (e.g., calibrate a model for the forecast site, install *in situ* sensors, identify which software or protocols will be used for forecast automation; Fig. 1 Step C), and begin obtaining input and validation data for forecasts (Fig. 1 Step D). Before forecasts are generated, the uncertainty associated with the forecast should be quantified so that a level of confidence in predictions can be communicated to end users (Fig. 1 Step E), and the most recent observational data can update the model (i.e., data assimilation; Table 1) so that the model is as closely aligned with current conditions as possible (Fig. 1 Step F). Finally, a forecast is generated (Fig. 1 Step G), disseminated to end users (Fig. 1 Step H), assessed with observations when data become available (Fig. 1 Step I), and the cycle begins again by seeking end user feedback to help assess the forecast and forecasting workflow (Fig. 1 Step A).

A key component of the near-term iterative forecasting cycle, which distinguishes forecasts from model predictions, is incorporating, quantifying, and reporting the uncertainty associated with estimates of future ecosystem states (Jakeman et al., 2019; Reggiani et al., 2022).

Uncertainty in near-term freshwater forecasts can arise from a variety of sources (Table 1), including uncertainty in forecasted model driver variables (e.g., error in the weather forecasts which serve as model input for a river flow forecast); uncertainty due to the forecast model structure's inability to fully represent the complex, real-world processes influencing the target forecast variable; uncertainty in model parameter estimates, and uncertainty in estimates of current (initial) conditions used as the starting point for running forecast models (Jakeman et al., 2019). When a forecast is produced, these uncertainties propagate (e.g., error in forecasted model driver variables leads to error in forecast model output; Table 1), resulting in increased uncertainty as the forecast progresses farther into the future (Dietze, 2017). Specifying the uncertainty associated with a model's prediction of future conditions, summed from the error sources described above and their interactions, facilitates informed decision-making by forecast end users.

Once a forecast has been generated and disseminated (Fig. 1 Steps G, H), there are many ways in which forecast accuracy and uncertainty can be assessed (Fig. 1 Step I; see Table 2 for examples of metrics developed to compare forecasts to observations and assess forecast uncertainty). In addition to comparing forecasts to observations, evaluation of forecasts using simple null or "naive" models (e.g., Perretti et al., 2013; see Table 1) has been identified as a best practice to test whether the chosen forecast model outperforms forecasts that assume the world is static (Harris et al., 2018; Lewis et al., 2022; White et al., 2019), i.e., whether the forecast provides a benefit. For example, a naive model might assume that tomorrow's conditions will resemble today's conditions with added noise (persistence forecast), or that they will be the same as a running average of that day-of-year's conditions from the past ten years ("climatology" or historical mean forecast; Jolliffe & Stephenson, 2012). Finally, a newly developed forecasting model can also be compared to the previously best-performing forecasting model for a specific target variable (e.g., Jin et al., 2019).

While the forecasting cycle (Fig. 1) represents best practices in near-term iterative forecasting (*sensu* Lewis et al., 2022), not all forecasting systems implement each step. For example, near-term freshwater forecasts can be characterized depending on whether the forecast is produced with data assimilation (Fig. 1 Step F; Table 1). Data assimilation (Table 1) can be conducted in multiple ways: e.g., by refitting a forecast model with the most recent observations, directly updating the initial conditions of the model to match recent observations, or using a statistical technique such as an ensemble Kalman filter or particle filter (Table 1) to adjust model predictions to be consistent with recent observations given uncertainty in both model predictions and observations (Cho et al., 2020; Dietze, 2017). Data assimilation has been shown to improve the accuracy of freshwater predictions (Cho et al., 2020), so has much potential for improving forecast usability, but is also computationally intensive and requires cyberinfrastructure for connecting data to models for real-time forecasting.

Another way forecasting systems can be characterized is by their workflows (Fig. 1 Step C). Forecast workflows can either be manual (i.e., steps in the iterative forecasting cycle are completed by a human) or automated (i.e., steps are triggered via cyberinfrastructure and occur without human intervention), depending on the goals of the forecasting project, forecast horizon, and frequency of data assimilation. For example, data ingest, defined as the process of making data accessible to the model (Table 1), can be done manually (e.g., a researcher digitizes new data; White et al., 2019) or it can be automated (e.g., sensor data are wirelessly streamed to a server and assimilated into the forecast model via cloud computing; Daneshmand et al., 2021). Other components of forecast workflows, including running models, creating forecast visualizations, and disseminating forecasts to end users, can also be automated (e.g., Baracchini et al., 2020). Automated, iterative workflows are often necessary for generating operational freshwater forecasts, defined as forecasts that are routinely produced and disseminated to the public and other end users (Table 1; e.g., Ayzel, 2021; Emerton et al., 2018; Fry et al., 2020; Nicolle et al., 2020). Manual forecast workflows are sometimes produced in academic settings as a tool for answering freshwater science research questions (e.g., Zwart et al., 2019), model testing, or when the temporal frequency of data collection and analysis is low enough or the forecast horizon is long enough (seasonal to annual forecasts) that automated, iterative workflows are not needed (e.g., Messager & Olden, 2018). For example, if a forecasting system is making 1 to 10-year-ahead forecasts of freshwater fish abundance using models run on an annual time step, there is likely no need for an automated system; in contrast, if a forecasting system is making hourly forecasts of floods, an automated iterative workflow would likely be critical.

The near-term iterative forecasting cycle (Fig. 1) can also be applied to predictive approaches which are critical for supplementing, advancing, and supporting forecasting system development and operation. In particular, hindcasting and model projections can be highly informative for developing near-term freshwater forecasts and informing freshwater decision-making (Table 1; Dietze, 2017; Jolliffe & Stephenson, 2012). Hindcasting, defined as developing forecasts for a time period which has already occurred (Jolliffe & Stephenson, 2012), is often done to test new forecast models (Kelley, 2022) or apply forecast models in new ecosystems (Woelmer et al., 2022). In practice, the only necessary difference between forecasting and hindcasting workflows is that the date for which the prediction is produced is either in the future (forecast) or the past (hindcast); all other components of the workflow (e.g., data assimilation, propagation of uncertainty) could be identical. In comparison, model projections run models into the future using a set of underlying assumptions or scenarios, thereby predicting a future predicated on specific conditions. For example, Lewandoski & Brenden (2022) developed model projections of whether continued lampricide application at historical levels would achieve invasive sea lamprey suppression targets in Lake Superior, USA by 2040. While projections can provide preemptive decision-making guidance, they cannot be used to make probabilistic statements about future events (unlike forecasts or hindcasts) since it is unknown which scenario is most likely to occur (Dietze, 2017). Hindcasting and model projection techniques can also be combined for assessing possible alternative management actions. For example, Bourgeaux et al. (2022) produced projections for a past time period to assess whether managed water releases from a floodplain lake could have achieved a lake escapement target to downstream habitat for threatened European eels.

Water quantity vs. water quality forecasting

Near-term forecasting of freshwater *quantity* (e.g., runoff, discharge, water level) has been a focus within hydrology for decades (Jain et al., 2018; Troin et al., 2021). Progress in water quantity forecasting has been motivated by the substantial risk to human health and property posed by both flooding and drought, which have both become more acute under global change (Han & Coulibaly, 2017; Jain et al., 2018; Kikon & Deka, 2022). These risks have prompted the creation of government-supported agencies and public and private centers to support water quantity forecasting at local, regional, national, and international scales (Troin et al., 2021) and grassroots communities of practice focused specifically on water quantity forecasting (e.g., Schaake et al., 2007). These communities facilitate interdisciplinary collaboration, knowledge transfer, and subsequently enable application of water quantity forecasting techniques at new sites.

Development of robust forecast systems for water quantity have been enabled in many cases by long-term government funding for sensor networks (Gunn et al., 2014) and well-established modeling approaches (Han & Coulibaly, 2017; Kikon & Deka, 2022; Mosavi et al., 2018; Troin et al., 2021). As a result, many water quantity forecasts are now automated and disseminated to water managers and the public at scales ranging from individual rivers or reservoirs to national and global scales (e.g., Ayzel, 2021; Baracchini et al., 2020; Emerton et al., 2018; Fry et al., 2020; Nicolle et al., 2020). Robust water quantity forecast systems have in turn enabled assessment of forecast economic value and utility to managers in various ways, including identifying which reservoir inflow forecast horizons are most useful to managers (Turner et al., 2020), estimating profit for farmers following forecast-informed water allocation (Giuliani et al., 2020), and assessing managers' ability to use streamflow forecasts to achieve a target reservoir level (Turner et al., 2017).

To date, the creation and public dissemination of freshwater *quality* forecasts have been less common than for water quantity. While much effort has been dedicated to prediction of select water quality variables, e.g., cyanobacterial density (Rousso et al., 2020) or water temperature (Baracchini et al., 2020; Ouellet-Proulx, St-Hilaire, et al., 2017; Sadler et al., 2022; Zhu & Piotrowski, 2020), agency- and/or center-based support and routine dissemination of water quality forecasts lags behind flood and stream/river discharge forecasting.

However, recent developments suggest that freshwater quality forecasting may catch up to water quantity forecasts in the near future. For example, the development of water quality monitoring sensor networks and the ability to wirelessly stream water quality data to the cloud

(Hestir et al., 2015; Marcé et al., 2016) permit updating of forecast models and forecasts in more remote locations and at higher resolution than was previously possible. Moreover, development of freshwater quality forecasts to inform natural resource management is now a priority for some government agencies (e.g., Bradford et al., 2020; NOAA, National Oceanic and Atmospheric Administration, 2014). Concurrently, interdisciplinary communities of practice, such as the Ecological Forecasting Initiative (Dietze & Lynch, 2019), are enabling idea generation and knowledge transfer among forecasters that could be used to advance the accuracy and utility of freshwater quality forecasts.

In sum, freshwater *quality* forecasting may be poised to advance rapidly in the near future, but the extent to which freshwater quality forecast workflows, methods, and accuracy compare to freshwater *quantity* forecasting remains unknown. To assess the field of near-term freshwater forecasting, we conducted a state-of-the-art literature review (*sensu* Grant & Booth, 2009) to synthesize and quantify recent progress in near-term forecasting of freshwater *quality*. We specifically focused on water quality as an emerging field within ecological forecasting to examine the progress in freshwater quality relative to freshwater quantity to date as well as identify potential future opportunities and challenges to overcome. Our questions centered around three focal areas:

I. **Forecast variables, scales, models, and accuracy:** Which freshwater variables and temporal scales are most commonly targeted for near-term forecasts, and what modeling methods are most commonly employed to develop these forecasts? How is the accuracy of freshwater quality forecasts assessed, and how accurate are forecasts? How is uncertainty typically incorporated into water quality forecast output?

II. **Forecast infrastructure and workflows:** Are automated, iterative workflows commonly employed in near-term freshwater quality forecasting? How often are forecasts validated and archived?

III. **Human dimensions of forecasts:** What are the stated motivations for creating near-term freshwater quality forecasts, and who are the most common end users (if any)? How are end users engaged in forecast development?

Below, we present our findings for each of these focal areas. We then synthesize across the focal areas with recommendations to advance the accuracy and scope of near-term freshwater quality forecasts and their utility to resource managers and other end users in an era of global change.

Materials and Methods

We conducted a state-of-the-art literature review (*sensu* Grant & Booth, 2009) of freshwater forecasting to assess the state of the field, recent progress, and ongoing challenges (see Text S1 and Fig. S1 for detailed methods). First, we conducted a search for peer-reviewed literature published in the last five years (since 1 January 2017) that included four key concepts (freshwater, forecasting, freshwater forecast target variables, and a combined resource management/global change concept) using the Web of Science™ Core Collection database (see Text S1 and Table S1 for detailed methods). All papers were accessed before 17 February 2022.

Second, we conducted a title screen for relevance, followed by an initial screen of papers. During the initial screen, we assessed whether: 1) the paper presented a prediction into the future from the perspective of the model (meaning no environmental observations were used as model input during the future prediction period); 2) the timescale of the prediction was near-term (minimum forecast horizon ≤ 10 yr; see Table 1 for definition of forecast horizon) or long-term;

3) the prediction was a forecast, hindcast, or projection and included uncertainty; 4) the target variable was freshwater *quantity* or *quality*. We also assessed the modeling approach for each paper, which we classified following Table 2. We then filtered our results to near-term forecasts, hindcasts, or projections with uncertainty of water quality variables. We included hindcasts and projections in addition to forecasts because: 1) the iterative, near-term forecasting cycle can be applied to all three predictive approaches; 2) both forecasts and model projections were used for freshwater management decision-making; and 3) we found that differentiating between forecasts and hindcasts was often not possible based on the information presented in peer-reviewed papers or their supplementary materials.

Third, we further analyzed each paper's near-term freshwater quality forecast, hindcast, or projection with uncertainty using a standardized matrix (Table S2) that addressed our focal research questions. Finally, we used the data from both our initial screen and in-depth water quality forecast analysis to assess the state of freshwater forecasting and identify areas of recent progress and ongoing challenges (see Text S1: *Literature review methods* for further details).

All data from the state-of-the-art literature review are available in the Environmental Data Initiative Repository (Lofton et al., 2022b) and all analysis-related code is published in the Zenodo repository (Lofton et al., 2022a).

Two important caveats to our review are that operational near-term freshwater quality forecasts produced by government agencies and private entities may not be routinely published in peer-reviewed articles, and that not all forecasting-relevant research results in production of near-term forecasts. For example, the United States (U.S.) National Oceanic and Atmospheric Administration (NOAA) provides both annual forecasts of cyanobacterial bloom intensity (Stumpf et al., 2016) as well as near-term bloom position predictions for Lake Erie (U.S. NOAA, Center for Operational Oceanographic Products and Services, 2018), but neither of these products were retrieved by our literature search. Moreover, in select cases information on operational near-term water quality forecast workflows may not be published for water security reasons, e.g., risk of cyberattack on water distribution infrastructure (Housh & Ohar, 2018). Finally, papers may report research that is important for advancing near-term freshwater quality forecasting but does not actually produce a forecast (e.g., Sadler et al., 2022; Zwart et al., 2019).

Results

I. Forecast variables, scales, models, and accuracy

Our literature search retrieved 963 papers, of which 507 were identified as describing future predictions of freshwater variables during our initial screen. While our focus was on water quality as described above, we analyzed all 507 “freshwater prediction papers” to compare the fields of freshwater quality vs. quantity (Fig. 3).

Water quantity dominates current freshwater prediction efforts

Water *quantity* variables (defined as lake or reservoir inflow, stream or river discharge, water level, or flood risk) were much more commonly predicted than any other freshwater variables (83%, n=424 of 507 freshwater prediction papers; Fig. 3). The vast majority (94%) of these 424 water quantity papers presented predictions at near-term (minimum forecast horizon ≤ 10 yr) timescales (Fig. 3). However, 50% of water quantity prediction papers (n=214 of 424) did not include uncertainty associated with predictions (Fig. 3).

Machine learning models (n = 191 of 424 papers) and ecosystem simulation models (n = 130) were the most frequent model types identified among papers presenting water quantity predictions (Fig. S2; see Table 2 for model type definitions). Machine learning models were the most common (140 of 231; 61%) model type in papers presenting near-term water quantity predictions without uncertainty, while simulation models were the most common (88 of 235; 37%) model type for predictions presented with uncertainty (Fig. S2). Simulation models were also the most popular choice (n = 18 of 27) among long-term (minimum horizon > 10 yr) water quantity predictions (Fig. S2). While most papers presented only one modeling approach, 13% of the water quantity prediction papers (n = 57 of 424) employed more than one modeling approach, with machine learning and empirical models being most commonly used in the same paper (n = 20 papers).

Water quality predictions target diverse ecosystem variables

The 16% of papers (n=83 of 507 freshwater prediction papers) predicting a water *quality* variable targeted a wide diversity of water quality metrics (Fig. 4). Popular target variables spanned physical water quality metrics (e.g., water temperature, n = 13 papers; sediment/turbidity, n = 9), chemical metrics (e.g., dissolved oxygen, n = 13; phosphorus or nitrogen concentrations, n = 10; conductivity/salinity, n = 8), and biological metrics (e.g., fish abundance or distribution, n = 11; phytoplankton abundance, n = 8; Fig. 4). Among water quality prediction papers, 64% (53 of 83 papers) did not incorporate uncertainty.

Most freshwater quality predictions are near-term

The majority (73%; n = 61 of 83) of water quality papers presented predictions at near-term (minimum forecast horizon ≤ 10 yr) timescales (Fig. 3). Papers presenting water quality predictions at long-term horizons more often included uncertainty compared to those presenting water quality predictions at near-term horizons (64% vs. 26%, respectively; Fig. 3). Altogether, 16 out of the 507 papers presented near-term water quality forecasts, hindcasts, or projections with uncertainty and were analyzed using our standardized matrix (Fig. 3; Table S3).

Among the 16 identified near-term water quality forecasts, hindcasts, or projections with uncertainty, minimum forecast horizons ranged from sub-daily (4 hr) to decadal (10 yr), with 3 papers presenting a maximum forecast horizon >10 yr (Fig. 5; Table S3). Papers presenting water quality forecasts, hindcasts, or projections for lotic ecosystems tended to either have daily (<7 days) or decadal (≥10 yr) maximum horizons, while forecasts in lentic ecosystems had horizons ranging from daily to monthly (30 – 365 days) scales (Fig. 5). There was no observable pattern relating the type of water quality target variable (physical, chemical, biological, or multiple) to maximum forecast horizon (Fig. 5).

Multiple modeling methods are being used to predict freshwater quality

Machine learning models (n = 34 of 83 papers), ecosystem simulation models (n = 22), and empirical models (n = 22) were the most frequent model types identified among papers presenting water quality predictions (Fig. S2; see Table 2 for model type definitions). Similar to water quantity prediction papers, machine learning models were the most common model type in papers presenting near-term water quality predictions without uncertainty, while simulation models were the most common model type for near-term water quality predictions presented with uncertainty (Fig. S2). Empirical models (defined in Table 2) were most often used for long-term water quality predictions (Fig. S2). Ten percent of water quality prediction papers (n = 8 of 83) employed more than one modeling approach. However, we found that only five of 16 near-term freshwater quality forecasting papers compared two or more models, with only three papers comparing the primary forecast model to a null model (defined as a persistence, historical mean, or first-order autoregressive forecast; Fig. 6).

Water quality forecast accuracy is usually assessed, but comparison of forecasts is challenging

Due to the wide variety of forecast target variables and assessment metrics presented among the near-term water quality papers we reviewed, we evaluated forecast accuracy (defined in Table 1) based on the metrics provided by the authors in each paper. Five of 16 water quality papers did not present a quantitative assessment of forecast accuracy. Of those that did provide quantitative assessment, root mean square error (RMSE; Table 2), reliability diagrams (Bröcker & Smith, 2007; Table 2), and continuous ranked probability score (CRPS; Table 2) were the most commonly employed assessment metrics (Fig. 6).

Across studies, forecast accuracy varied among target variables and forecast horizons (Table 3). Three studies forecasting reservoir and river water temperature reported CRPS < 1.1^{o} C (see Table 2 for definition and interpretation of CRPS) for forecast horizons from one to 16 days into the future (Table 3; Ouellet-Proulx, Chimi Chiadjeu, et al., 2017; Ouellet-Proulx, St-Hilaire, et al., 2017; Thomas, Figueiredo, et al., 2020). An additional study reported greater accuracy in seasonal (one- to four-month-ahead) forecasts of bottom water temperatures compared to surface waters across four lakes and reservoirs in Spain, Norway, Germany, and Australia (Table 3; Mercado-Bettín et al., 2021), which the authors attributed to greater thermal inertia in the bottom waters of lakes. Two studies provided forecasts of nitrogen (N) and phosphorus (P) concentrations (NH_4-N, NH_3-N, total N, total P), with a reported bias (Table 2) ranging from 0.001 to 0.028 mg L^{-1} for 0 – 5 days ahead (Peng et al., 2020) and a reported RMSE of 0.0487 mg L^{-1} for one-day-ahead forecasts of NH_3-N concentrations (Table 3; Jin et al., 2019). Forecasts of lake dissolved oxygen concentrations (bias = 0.008 – 0.022 mg L^{-1} for 0 – 5 day lead times; Peng et al., 2020), lake methane ebullition emissions (RMSE = 0.48 – 0.53 ln(mg CH4 m^{-2} d^{-1}) for one- and two-week lead times; McClure et al., 2021), river turbidity (RMSE = 0.0024 NTU for one-day-ahead forecasts; Jin et al., 2019), and river conductivity (RMSE = 0.0068 μS cm^{-1} for one-day-ahead forecasts; Jin et al., 2019) were reported by one study each (Table 3).

While three studies presented near-term forecasts of phytoplankton-related variables in lakes, differences in their methodology precluded comparison. Two studies assessed their forecasts by converting the forecast to binary predictions (occurrence/non-occurrence of a bloom event; Mu et al., 2021) and exceedance/non-exceedance of a cyanobacterial toxin concentration threshold Liu et al., 2020), both of which reported better-than-chance skill at forecast horizons up to 5 – 7 days ahead (Table 3). One additional study provided probabilistic forecasts of chlorophyll-a concentrations in two English lakes, with a reported RMSE of ~2.75 – 5.25 mg m^{-3} for 1–10 days ahead over three years at one lake, and an RMSE of ~8.25 – 17 mg m^{-3} for 1 – 10 days into the future over two years at the second lake (Table 3; Page et al., 2018).

Less than half of water quality predictions incorporate uncertainty

Notably, only 36% of papers (30 of 83) that presented predictions of freshwater quality variables into the future incorporated uncertainty (Fig. 3). Within near-term water quality forecasts, hindcasts, and projections with uncertainty (n = 16), multiple methods of uncertainty specification were employed. For example, some papers included the concept of uncertainty but did not quantify it (e.g., used different land use change scenarios as model drivers; Chen et al., 2020; these papers were categorized in the “present” category for uncertainty inclusion methods following Table 2) whereas others quantified and propagated uncertainty while also iteratively assimilating new observations to constrain initial conditions (e.g., Baracchini et al., 2020; Liu et al., 2020; these papers were categorized in the "assimilates" category for uncertainty inclusion methods following Table 2; Fig. 6). Of the sixteen near-term freshwater quality prediction papers that reported uncertainty, four were projections and 12 were forecasts or hindcasts. A majority (n = 7 of 12) of near-term freshwater quality forecasts and hindcasts both propagated uncertainty and assimilated new observations (Fig. 6). All papers presenting projections were categorized as having uncertainty "present" or "data-driven" (i.e., not propagating uncertainty or assimilating new observations; see Table 2 for definitions of uncertainty categories).

II. Forecast infrastructure and workflows

Overall, while most of the near-term freshwater quality forecasts we analyzed were generated using the iterative forecasting cycle framework (n = 11 of 16; Fig. 1, Table S3), only three papers representing two forecasting systems reported producing forecasts via automated workflows (Baracchini et al., 2020; Carey et al., 2022; Thomas, Figueiredo, et al., 2020). In both cases, the authors described automated forecast workflows that included the steps of: 1) retrieval of new observational data and meteorological forecasts to force a freshwater ecosystem forecasting model; 2) assimilation of observational data to inform model initial conditions and parameters; 3) model runs; and 4) delivery of the automated forecast to end users via a web interface or other web-based communication (Baracchini et al., 2020; Carey et al., 2022; Thomas, Figueiredo, et al., 2020).

Archiving forecasts was also not a commonly-reported practice among forecast papers. Three papers reported archiving of forecasts, either by publishing data and forecasts retroactively to a data repository upon publication of the associated paper (McClure et al., 2021) or providing them in real time via an open online platform or repository (Baracchini et al., 2020; Carey et al., 2022). In two cases, authors reported that the forecast-related code was also published with a digital object identifier (DOI; Carey et al., 2022; McClure et al., 2021). We note that information on infrastructure and workflows may be difficult to extract from academic research papers as the focus is often on forecast results and performance rather than methodology. In addition, as noted above, operational forecast workflows developed by government agencies or private entities may not be published in academic journals, or the availability of these workflows may be limited by ethical considerations or security concerns (Hobday et al., 2019; Housh & Ohar, 2018).

III. Human dimensions of forecasts

Water quality forecasts are motivated by ecosystem services and increased variability

The development of many of the near-term freshwater quality forecasts we analyzed was motivated by the need for freshwater ecosystem services in the face of increased ecosystem variability due to global change (Fig. 2). Researchers identified increased variability in management-relevant ecosystem variables such as water temperature (Carey et al., 2022; Thomas, Figueiredo, et al., 2020), distribution of freshwater fishes (Fraker et al., 2020), invasive species (Messager & Olden, 2018), and algal biomass (Liu et al., 2020; Mu et al., 2021; Page et al., 2018) as motivation for forecast development. In all cases, the stated motivation for anticipating increased variability was coupled with a desire to preemptively inform freshwater management and decision-making. Indeed, improving freshwater resource management was stated as motivation for forecast development in every freshwater quality forecast paper we analyzed (see Table S3 for complete list), save one (McClure et al., 2021). In addition to providing early warnings to resource managers and the public under global change, researchers mentioned improving forecasting methodology (Bhattacharyya & Sanyal, 2019; Peng et al., 2020) and understanding of ecological processes (McClure et al., 2021) as additional factors motivating forecast development.

End user engagement not often reported in water quality forecast papers

Despite that nearly all freshwater quality forecast papers stated improved water resource management as motivation for forecast development, only six of 16 papers, representing four distinct forecast systems, named any forecast end users (Baracchini et al., 2020; Carey et al., 2022; Liu et al., 2020; Ouellet-Proulx, Chimi Chiadjeu, et al., 2017; Ouellet-Proulx, St-Hilaire, et al., 2017; Thomas, Figueiredo, et al., 2020). These four forecast systems generated predictions for a small, temperate drinking water reservoir (Falling Creek Reservoir, U.S.; Carey et al., 2022; Thomas, Figueiredo, et al., 2020), a large north temperate lake (Lake Geneva, Switzerland; Baracchini et al., 2020), two north temperate rivers (Miramichi and Nechako Rivers, Canada; Ouellet-Proulx, Chimi Chiadjeu, et al., 2017; Ouellet-Proulx, St-Hilaire, et al., 2017), and a Laurentian Great Lake (Lake Erie, U.S.; Liu et al., 2020). Incorporation of end users ranged from briefly mentioning that end users were associated with a particular forecast site or variable (Liu et al., 2020; Ouellet-Proulx, Chimi Chiadjeu, et al., 2017; Thomas, Figueiredo, et al., 2020) to detailing multiple mechanisms for engaging end users in forecast development (Carey et al., 2022). Carey et al. (2022) described co-developing a water quality forecast with drinking water reservoir managers in southwest Virginia, U.S. by: 1) working with managers to identify useful target variables for forecasting; 2) observing water treatment plant operations to better understand managers' daily activities; and 3) requesting feedback on forecast visualizations to improve their use for decision-making. Ouellet-Proulx, St-Hilaire et al. (2017) also provide a specific management motivation for their target variable of water temperature: helping lake managers in British Columbia, Canada plan summer water releases to reduce thermal stress for downstream freshwater fish.

While most papers focused on resource managers as potential end users or did not specify end user identity, one paper did report on how forecasts were used by multiple user groups. Baracchini et al. (2020) documented the use of their hydrodynamics and water temperature forecast system by various members of the community surrounding Lake Geneva, Switzerland using data collected from their forecast dissemination website. The authors were able to verify forecast use and acceptance by the community (evidenced by ~1000 visitors to their website per day in summer 2019) and to differentiate three types of end users: scientists, lake professionals, and the public. While end user engagement was infrequently reported in near-term water quality forecast papers, it is possible that forecast teams were engaging end users but not reporting it, especially if the focus of the paper was to document other aspects of the forecast system, such as model development or forecast accuracy.

Discussion & Synthesis: Opportunities to advance near-term freshwater quality forecasting

Our findings indicate that the majority of near-term water quality forecasts published as peer-reviewed articles in the past five years are in an early stage of development, serving as "proofs-of-concept" rather than as operational forecasts. These results set the stage for additional work to be done before water quality forecasting catches up with water quantity forecasting. Nonetheless, the papers we analyzed demonstrate key areas of recent progress that will be critical to future development of operational near-term freshwater quality forecasts, including:

quantitative, probabilistic forecasts of both abiotic and biotic variables (e.g., Jin et al., 2019; Liu et al., 2020; Page et al., 2018; Peng et al., 2020), forecasts at management-relevant time horizons (e.g., Mercado-Bettín et al., 2021), use of probabilistic forecast assessment metrics (e.g., Ouellet-Proulx, Chimi Chiadjeu, et al., 2017; Ouellet-Proulx, St-Hilaire, et al., 2017), comparison of forecasts to null models (e.g., McClure et al., 2021; Page et al., 2018; Thomas, Figueiredo, et al., 2020), uncertainty propagation and partitioning (e.g., McClure et al., 2021; Thomas, Figueiredo, et al., 2020), iterative, automated workflows (e.g., Baracchini et al., 2020; Thomas, Figueiredo, et al., 2020), co-development of forecasts with end users (e.g., Carey et al., 2022), and assessment of forecast use by a range of end users (e.g., Baracchini et al., 2020). Further advances in near-term freshwater quality forecasting will require continued development of forecasting tools and skills as well as more substantive end user engagement (Fig. 2).

Here, we synthesize the results from the review to provide a list of seven recommendations comprising an agenda for developing the next generation of near-term freshwater quality forecasts, with an emphasis on building automated, operational forecast systems (Fig. 2).

1. A definition of forecast that includes uncertainty

All forecasts are inherently uncertain as perfect knowledge of future events is impossible, and therefore a forecast should, by definition, specify uncertainty (Fig. 2: quantified uncertainty; uncertainty specification, propagation, and analysis). Underestimation of forecast uncertainty or omission of uncertainty from predictions can lead to overconfidence in forecast accuracy, potentially affecting management decisions based on forecast output (Berthet et al., 2016). One compelling example of the risks associated with omission of uncertainty from predictions is the

1997 Red River flooding event in Grand Forks, ND, U.S. and East Grand Forks, MN, U.S., when the U.S. National Weather Service's prediction of a 49 ft flood crest (with no quantitative uncertainty estimate associated with the flood crest height prediction) was incorrectly interpreted by decision-makers, leading to inundation and tremendous flood damage when dikes to protect the cities failed (Pielke, 1999).

In addition to improving decision-making outcomes, uncertainty quantification and partitioning (Table 1) can inform the most effective ways to improve forecast accuracy (e.g., Lofton, Brentrup, et al., 2022). For example, if uncertainty partitioning identifies that forecast model driver data is the biggest source of forecast uncertainty, then reducing uncertainty in driver data would be a logical next step for improving that forecast system (following Thomas, Figueiredo, et al., 2020). Importantly, reducing uncertainty in a forecast does not necessarily improve forecast accuracy if the forecast is biased (e.g., tends to over- or underestimate), and metrics that assess forecasts based on the degree of forecast uncertainty (e.g., sharpness; Table 2) are often predicated on the assumption that the forecast is sufficiently accurate (Gneiting, Balabdaoui, et al., 2005). Furthermore, even forecasts for which uncertainty is robustly characterized may not capture all possible future outcomes if an outcome occurs due to processes not included in the forecast model or has no historical analogue (Boettiger, 2022; NRC, 2010; Thompson & Smith, 2019). For example, a lake water quality model will likely fail to accurately predict future water quality if a new species that is not represented in the model invades the lake and alters water quality (e.g., an unexpected invasion of the spiny water flea, *Bythotrephes longimanus*; Walsh et al., 2016).

Despite the importance of incorporating uncertainty into future predictions, our review revealed that only 36% of papers predicting freshwater quality variables into the future specify uncertainty. Our findings highlight an opportunity for more robust specification and partitioning of uncertainty in freshwater forecasting efforts. Importantly, some freshwater forecasters are already successfully employing sophisticated uncertainty specification techniques, evidenced by the 7 of 12 near-term water quality forecasts and hindcasts which both propagate uncertainty and assimilate new observations to inform model initial conditions (Fig. 6).

Importantly, while we included all methods of representing uncertainty in predictions in our review, some methods of specifying uncertainty are likely to be more useful to freshwater forecast end users than others. For example, if a manager is presented with a projection that includes uncertainty by running a model with multiple scenarios (e.g., different levels of capture effort for an invasive crayfish, such as 50, 100, or 200 person-hours per week dedicated to crayfish capture within a stream network over the next five years) but a range of uncertainty *within* each scenario is not specified, that projection effectively becomes a deterministic prediction with no uncertainty once a management decision is made (e.g., a capture effort of 100 person-hours per week, represented by one possible scenario, is selected). If uncertainty were quantified *within* each scenario, a manager could evaluate the probability of achieving a desired outcome *given* a particular management action (e.g., a capture effort of 100 person-hours per week has a 90% probability of reducing crayfish abundance to < 1 crayfish m^{-2} in five years). Considering how a forecast or projection will be used for decision-making should guide methods for quantifying uncertainty in freshwater quality predictions.

2. Integration of end users into the forecast process

Freshwater quality forecasts are developed by people, for people, and to date have been primarily intended for use by freshwater managers. It follows that formation of forecaster-manager partnerships should be integral to forecast development, and that managers and other end users should be engaged throughout the forecast process (Fig. 2: end user engagement). For example, during the early stages of forecast system development, end users can identify which target forecast variables are most useful (e.g., asking ship captains whether forecasts of lake ice concentration or ice thickness are more useful; Fujisaki-Manome et al., 2022), and over which time horizons forecasts should be provided (DeFlorio et al., 2021; Turner et al., 2020). During model development, expert elicitation, a formal process of extracting expert knowledge while mitigating bias (Hemming et al., 2018), can be employed to inform model structure (e.g., Bertone et al., 2016). End users should also be consulted regarding forecast dissemination methods to ensure correct interpretation of forecast output and maximize forecast utility (Berthet et al., 2016; Gerst et al., 2020; Theocharis & Smith, 2019). For example, interviews and focus groups with end users of NOAA's Climate Prediction Center climate outlook visualizations guided updates of NOAA's air temperature and precipitation color maps for improved forecast interpretability (Gerst et al., 2020). Finally, feedback from managers and end users should be sought after forecast dissemination to determine if the forecast product is being successfully implemented for decision-making support (e.g., Jackson-Blake et al., 2022).

Of the 16 near-term freshwater quality forecasting papers analyzed, two emphasized end user engagement, specifically co-development of forecasts with resource managers (Carey et al., 2022) and assessment of forecast acceptance and use (Baracchini et al., 2020). These examples illustrate the potential for co-development of additional operational freshwater quality forecasts suitable for management decision-making in the near future.

3. More forecasts using diverse modeling approaches over multiple horizons

Advances in freshwater quality forecasting require the existence of initial forecast systems upon which to improve, serving as precursors for operational near-term water quality forecast systems (Fig. 2: operational, near-term water quality forecasts). The dominance of water *quantity* predictions (83% of freshwater prediction papers) over water *quality* predictions in our literature review underscores the critical need for developing additional near-term freshwater quality forecasts, ideally using diverse modeling approaches over multiple forecast horizons. The wide diversity of water quality forecast target variables in our review (Fig. 4) highlights that for any individual target variable, relatively few forecasts are being produced, limiting intercomparison of forecasting approaches.

Forecasts of a single target variable using multiple modeling techniques at many sites (e.g., Sadler et al., 2022) are needed to produce actionable forecasts and provide insight on freshwater ecosystem function. Employing a wide diversity of modeling approaches is necessary to avoid the "forecast trap" (*sensu* Boettiger, 2022), wherein the most accurate available forecast does not lead to an optimal management outcome. The trap arises when the range of possible outcomes predicted by an ensemble of models is too narrow, providing managers with insufficient guidance about how their decisions might manifest in the real world (Boettiger, 2022; Thompson & Smith, 2019). Moreover, forecast end users typically integrate multiple forms of information when making decisions (e.g., Fujisaki-Manome et al., 2022). As a result, development of a diversity of both quantitative (e.g., tomorrow's dissolved oxygen will be 1.8 ± 0.5 mg L^{-1}) and categorical (e.g., the risk of observing hypoxia tomorrow will be *high*) forecasts that incorporate model output and human expertise (Tetlock & Gardner, 2016) will likely be needed to support a variety of forecast end users in achieving optimal management outcomes.

Importantly, forecasters should also consider both simple and complex model structures, as simple models may prove the most effective for forecasting certain variables, such as vertebrate population size forecasts (Ward et al., 2014), whereas complex process-based models may be better at forecasting conditions that fall outside of the envelope of historical conditions (Adler et al., 2020). Finally, comparison of more complex models against simple models (i.e., null or naive models) is necessary to quantify the benefit of added model complexity (e.g., Perretti et al., 2013).

In addition to employing diverse modeling approaches, production of forecasts at multiple time horizons is needed to ensure maximum forecast utility for end users. Different end user decisions are made at different time scales; for example, a ship captain may be most interested in lake ice conditions over the next several hours to days when deciding whether to embark (Fujisaki-Manome et al., 2022), while a reservoir manager may look multiple months ahead when planning water releases downstream (Jackson-Blake et al., 2022; Turner et al., 2020). We observed a relative dearth of near-term freshwater quality forecasts at multi-month/seasonal timescales (but see Mercado-Bettín et al., 2021; Fig. 5), highlighting an opportunity for development of additional forecasts at this horizon. Furthermore, assessment of forecasts across multiple horizons may lead to insights regarding the intrinsic predictability of freshwater ecosystems (*sensu* Pennekamp et al., 2019), in turn informing which modeling approaches are likely to be most successful for freshwater forecasting (Pennekamp et al., 2019; Petchey et al., 2015).

Development of forecasts of a single target variable at many sites with different environmental conditions can also provide insight on the intrinsic predictability of water quality and the utility of forecasting for water quality management across ecosystems. Initiatives such as the National Ecological Observatory Network (NEON) Ecological Forecasting Challenge (Thomas, Boettiger, et al., 2021), which solicits participants to submit forecasts for multiple sites using standardized data collected by NEON and assesses them for accuracy, are a starting point to compare predictability across ecosystems and model types (e.g., Thomas et al., 2022). However, the freshwater component of the NEON Challenge is limited to seven lakes and 27 streams occurring within the U.S., and therefore lacks a suitably wide range of environmental conditions to be globally relevant. Moreover, forecasts are evaluated for accuracy only, not for optimal management outcomes. Additional efforts to develop multi-site forecasts are needed to assess freshwater ecosystem predictability under global change as well as ensure maximum forecast utility for water quality management.

4. Shared standards for workflows, file formats, metadata, archiving, and benchmarking

Building better models is not sufficient to improve near-term freshwater quality forecast accuracy. Development of automated, portable, and reproducible workflows (e.g., Huang et al., 2019; White et al., 2019), standardized metadata and file formats (e.g., Dietze et al., 2021), repositories for archiving forecasts (e.g., Reich et al., 2021), and consensus on methods for benchmarking forecast accuracy (Dietze et al., 2018; Smith et al., 2015) are also needed (Fig. 2: automated, iterative workflows, archiving and metadata, forecast assessment).

Portable, reproducible workflows are characterized by the ability to replicate results whenever and wherever the workflow is run (e.g., avoiding the problem of obtaining a different result if a user's software has been updated or across different operating systems) and the ability to be easily accessed by users (Vaillancourt et al., 2020). Example of tools that facilitate development of portable, reproducible forecast workflows include software containers, which can package, for example, forecasting code with all the necessary dependencies and computing environment specifications into self-contained units for reproducible analyses (Cito et al., 2017) and cloud computing, which allows users to access, for example, forecast output from any device at a location and time of their choice, rather than requiring each user to have specialized infrastructure for running a forecast on a local computer (Sunyaev, 2020). The diverse landscape of constantly-evolving computing technologies available for use in water quality forecast workflows highlights the importance of 1) engaging interdisciplinary expertise in forecast development teams, including computer science (Carey et al., 2019, 2022) and 2) developing accessible, community-based cyberinfrastructure tools and software (Boettiger et al., 2015; Fer et al., 2021).

Standardized file formats for observational data, forecast output, and metadata (e.g., Dietze et al., 2021) facilitate automated assimilation of data into forecast models (e.g., Huang et al., 2019; White et al., 2019), regular dissemination of forecasts to end users (e.g., Baracchini et al., 2020; Daneshmand et al., 2021), and quantitative forecast inter-comparison. Shared community standards are critical for initiatives such as the NEON Ecological Forecasting Challenge to compare and score forecasts across sites of different variables submitted by participants (Thomas, Boettiger, et al., 2021). Additional efforts to produce intercomparable forecasts using shared standards are needed to advance freshwater quality forecasting. Adoption of standardized data formats and metadata by freshwater research networks such as the Global Lake Ecological Observatory Network (GLEON; Weathers et al., 2013) could facilitate freshwater quality forecasting by providing databases with which multiple forecasting approaches could be tested at the global scale. While some initiatives have begun this work (e.g., Jennings et al., 2017), the lack of wide-scale adoption of community standards hinders progress in freshwater quality forecasting.

Once file formats have been developed, archiving forecasts in real time promotes integrity in forecast benchmarking. For example, forecasts that are published in peer-reviewed manuscripts may be altered and re-run during the peer review process in response to reviewer feedback; if so, subsequent analysis of these forecasts for accuracy would not reflect the accuracy of the original forecasts that were available to end users in real time. However, the iterative nature of real-time forecast products raises several pertinent archiving challenges, including development of repositories that permit automated, iterative updating of forecast output as additional forecasts are produced, and whether and how to assign digital object identifiers (DOIs) to data products that will change or be updated every time a new forecast is issued. This is a problem that is not specific to freshwater forecasting, and recent efforts to develop a discipline-agnostic archive specifically designed for predictive products, with standardized data and metadata formats, scoring, and visualizations (Reich et al., 2021), illustrate that early integration of archiving into freshwater quality forecasting efforts could have long-term benefits for promoting forecast intercomparison.

In addition to formalizing community standards for data, forecast outputs, and archiving, freshwater forecasters need to build consensus on how to assess forecast accuracy (Pappenberger et al., 2015). The properties of candidate benchmark assessment metrics should be carefully considered to ensure that the desired attributes of freshwater quality forecasts (e.g., high accuracy) are adequately rewarded and undesirable attributes (e.g., large uncertainty spread) are penalized. For example, sharpness penalizes forecasts with a large uncertainty spread but does not assess the distance of a forecast prediction from the observation (Gneiting, Balabdaoui, et al., 2005; Table 2), while the ignorance score heavily penalizes forecasts that fall far from observations (Roulston & Smith, 2002).

Fortunately, freshwater quality forecasters are starting to adopt methods of forecast assessment that facilitate benchmarking and intercomparison of probabilistic forecasts. For example, adoption of a probabilistic forecast assessment metric (CRPS) by multiple water temperature forecasters enabled us to compare forecast accuracy for two forecasting systems in a reservoir and two rivers, respectively (Ouellet-Proulx, Chimi Chiadjeu, et al., 2017; Ouellet-Proulx, St-Hilaire, et al., 2017; Thomas, Figueiredo, et al., 2020). Based on the accuracy of these two forecasts, future forecasts of surface water temperature up to 16-days ahead could be benchmarked against a CRPS of ~1º C, the maximum CRPS observed in these studies. Other forecasters compared their forecasts to commonly-used null models (e.g., persistence models in both McClure et al., 2021 and Page et al., 2018), another robust method for benchmarking forecast accuracy (Harris et al., 2018). But overall, the wide variety of assessment metrics currently used to quantify water quality forecast accuracy (Fig. 6) makes inter-comparison of forecasts difficult. Efforts to reach consensus on appropriate methods for benchmarking other important water quality variables (e.g., dissolved oxygen, chlorophyll-a) are needed to measure improvements in near-term freshwater quality forecast accuracy over time.

5. Integration of insights from other forecasting disciplines

Near-term freshwater quality forecasting will benefit by integrating and adapting tools and skills from more mature forecasting disciplines, particularly weather, marine, and water quantity forecasting (Fig. 2: tools and skills). Arguably the largest and most mature Earth system forecasting discipline, weather and climate forecasting offers methodological inspiration and guidance to water quality forecasters on a number of fronts, including data assimilation (reviewed in Lahoz & Schneider, 2014), uncertainty quantification (e.g., Yip et al., 2011), and forecast assessment (e.g., Gneiting, Raftery, et al., 2005; Hersbach, 2000). For example, the CRPS probabilistic forecast metric, which was used in four of 16 near-term water quality forecasts identified in our review, has been used in weather forecasting for decades (Gneiting, Raftery, et al., 2005; Hersbach, 2000). In addition, examining the benefits and disadvantages of the numerous methods for public dissemination of weather forecasts, ranging from mobile phone applications (Zabini, 2016) to televised verbal interpretation by local, human forecasters (Compton, 2018), may be helpful for water quality forecasting teams to consider as they work to provide forecast output that meets end user needs. For example, mobile phone applications may provide the benefit of hyper-localized forecast information but lack the capacity for the user to put this information into a regional context (Zabini, 2016). Finally, the history of weather forecasting demonstrates that improvement in forecast skill over time is possible even if initial attempts are quite poor (Bauer et al., 2015; Blum, 2019), providing motivation to aspiring freshwater quality forecasters to begin forecasting now, even in the face of incomplete knowledge (Dietze et al., 2018).

Freshwater quality forecasters can also apply lessons learned from marine and water quantity forecasters regarding, e.g., model development (Varadharajan et al., 2022), forecast dissemination (Choi et al., 2022), and the ethical implications of providing operational forecasts (Hobday et al., 2019; Record & Pershing, 2021). Moreover, insights from marine and freshwater quantity forecasting may be particularly relevant to freshwater quality forecasting as all three disciplines involve aquatic ecosystems. For example, researchers are now applying machine learning methods long popular in freshwater *quantity* forecasting to water *quality* forecasting (reviewed by Poh Wai et al., 2022), and several challenges informed by use of machine learning models in water *quantity* have been identified, including the need for knowledge-guided machine learning, incorporation of uncertainty, transfer learning (i.e., models trained at data-rich sites are then applied at data-poor sites), and improved interpretability of model output (Khudhair et al., 2022; Poh Wai et al., 2022; Varadharajan et al., 2022). As another example, many of the lessons learned in development and dissemination of predictive water quality guidance at marine beaches may readily transfer to freshwater beaches, such as the utility of three-dimensional models for capturing diurnal fluctuations in water quality (Choi et al., 2022), methods for coordinating data collection among multiple agencies to assess urban water quality (Aznar et al., 2022), or the difficulty of developing adequate water quality predictive tools (e.g., *E. coli* predictions) for beaches subject to frequent visits by large flocks of birds (U.S. EPA, 2016). Finally, ethical considerations relevant for operational marine forecasts, such as the risk of driving lobster prices up or down based on lobster landing forecasts (Hobday et al., 2019), may have freshwater analogues, such as economic risks associated with providing freshwater fishery forecasts.

Forecasting techniques and ideas gleaned from other disciplines will likely require adaptation to account for unique attributes of water quality data and freshwater ecosystem processes before being applied in a freshwater quality forecasting context. However, recent innovations in freshwater quality forecasting methodology, including embedding freshwater-relevant physical processes into machine learning model architectures (Daw et al., 2020; Read et al., 2019) and data assimilation of multiple freshwater quality data streams with different attributes (Abdul Wahid & Arunbabu, 2022; Chen et al., 2021; Cho et al., 2020; Cobo et al., 2022), illustrate the benefits of adapting practices from other disciplines for water quality forecasting.

6. Financial support for near-term water quality forecasting

Most of the near-term freshwater quality forecasts that we analyzed are still in early stages of development, necessitating funding to support collection of data, development of automated, iterative workflows, advancement of modeling and uncertainty analysis methods, robust forecast archiving, and assessment of forecast accuracy and utility to managers (Fig. 2: funding support). Some freshwater quality forecasting efforts could leverage existing data collection programs run by agencies and sensor networks (e.g., NEON, U.S. Geological Survey); however, to date, there has been much more standardized sensor infrastructure investment in water *quantity* monitoring than *quality* monitoring.

Unprecedented efforts in freshwater prediction are underway, necessitating broad investments that span federal and state agencies as well as academic research portfolios. For example, the European Center for Medium-Range Weather Forecasts (ECMWF), along with the European Space Agency and the European Organization for the Exploitation of Meteorological Satellites, have launched Destination Earth, a project to create an interactive "digital twin" of Earth that will incorporate hydrology in addition to climate and land systems and can be used as a predictive tool (Nativi et al., 2021). In addition, Earth system predictability has been identified as a U.S. federal funding priority (Vought & Droegemeier, 2020). To date, water forecasting divisions or programs have been developed by several U.S. agencies, including the National Aeronautics and Space Administration (NASA; Arsenault et al., 2020) and National Oceanic and Atmospheric Administration (NOAA; U.S. NOAA, 2022). In addition, a new epidemiological forecasting center has just launched at the Centers for Disease Control (CDC; U.S. CDC, 2022). For each of these initiatives, freshwater quality forecasting can and should be explicitly identified as a priority to support essential agency mandates, whether in the context of supporting the Blue Economy (e.g., Petrea et al., 2021) or preventing waterborne disease outbreaks (e.g., Nusrat et al., 2022). Funding opportunities that explicitly encourage the cross-disciplinary collaboration required to build automated, operational forecasting systems with end user engagement will be most helpful in facilitating development of robust water quality forecast systems.

Importantly, indefinitely maintaining an operational forecast system is outside the scope of most academic research programs, as it requires infrastructure maintenance and investment in personnel extending beyond the timespan of most academic research grants (Carey et al., 2022; Hobday et al., 2019). As a result, additional funding will be required to facilitate transition of operational forecast systems from academic teams to industry and government agencies.

7. Further development of educational resources and communities of practice

Ultimately, generating accurate freshwater quality forecasts requires extensive training of the forecasting team. Obtaining training in a multi-disciplinary, emerging field like ecological forecasting can be challenging (Woelmer et al., 2021), motivating the need for broad sharing of educational materials (Moore et al., 2022; Willson, 2022) and open-source tools and software (e.g., Boettiger et al., 2015; Daneshmand et al., 2021; Hipsey et al., 2019; Moore et al., 2021) within active communities of practice (Fig. 2: educational resources; communities of practice). Communities of practice may occur within government agencies, originate from a specific project such as the Hydrological Ensemble Prediction Experiment (HEPEX; Schaake et al., 2007), take the form of grassroots networks such as the Ecological Forecasting Initiative (EFI; Dietze & Lynch, 2019), exist as formal professional societies, or be housed at academic institutions.

To help train new forecasters, forecasting communities of practice should help create and facilitate sharing of resources, such as teaching modules focused on fundamental forecasting concepts (Moore et al., 2022), curated lists of freely available forecasting educational resources (Willson, 2022), and community-based development of software (Boettiger et al., 2015). In addition, education in freshwater quality forecasting would be enhanced by introducing forecasting (and uncertainty) at earlier educational stages (e.g., in K-12 education; Rosenberg et al., 2022) and development of formal curricula in freshwater forecasting specifically (Moore et al. 2022).

Conclusions

Near-term freshwater quality forecasts are urgently needed as freshwater ecosystems are experiencing increasing variability on near-term timescales due to global change, causing substantial risk to human health and safety. Water quality forecasting is primed to make considerable advances over the next decade, as evidenced by a wide diversity of potential applications, end users of accurate water quality forecasts, and recent progress in forecasting methodology. Continued progress necessitates development of more forecasts: to robustly measure gains in forecast accuracy, we must be able to compare forecasts of the same variables across a wide diversity of sites, modeling approaches, and forecast horizons. Such a multi-faceted forecasting effort will require concomitant development of community standards regarding forecast metadata, file formats, archiving, and benchmarking to permit forecast intercomparison. Second, as we develop freshwater quality forecasts, we should avail ourselves of lessons learned in other forecasting disciplines, whether it be innovating methods of incorporating uncertainty into machine learning models adapted from water quantity forecasting or taking inspiration from the continuous improvement in weather forecast accuracy made over decades. Finally, we must remember that operational freshwater quality forecasts are developed by people, for people, and thus require both comprehensive training opportunities for forecasters and meaningful end user interaction throughout the forecast process. Given the promise of freshwater forecasting for improving management in the face of increased variability and risk due to global change, we urge freshwater scientists to engage with end users, assemble interdisciplinary teams, and get started on building operational near-term water quality forecasts.

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Tables

Table 1: Definitions and examples of terms related to freshwater forecasting. Definitions are adapted from multiple sources (Carey et al., 2022; Dietze, 2017a; Lewis et al., 2022; Lofton et al., 2022; McClure et al., 2021; Thomas & Figueiredo, 2020), with additional references for select terms provided in the table.

Term	**Definition**	**Freshwater quality example**
Automated workflow	A forecasting system that produces new forecasts on a set schedule or in response to another automated action and does not require a person to manually initiate forecast generation	A lake water temperature forecast that is triggered to be issued every six hours as new meteorological forecasts are available from US NOAA
Data assimilation	Updating either initial conditions, model states, and/or model parameters through statistical comparison of model predictions to new observations not previously ingested by the model	Using a Kalman filter to update initial conditions in a weekly forecast of algal biomass concentrations
Data ingest	The process of making data accessible to a model (e.g., for data assimilation)	Chlorophyll-a sensor data are wirelessly streamed to a server and assimilated into the forecast model on a daily time step
Ensemble	Repeated model runs using different values of parameters, initial conditions, driver data, and/or random processes	Running a model to predict tomorrow's zooplankton biomass 100 times using different draws from a distribution of possible zooplankton growth rate parameter values, possible current zooplankton biomass values, and possible forecasted water temperatures
Forecast	Predictions of the future state of a physical, chemical, or	There is a 45% chance that dissolved iron concentrations

	biological freshwater variable that incorporates uncertainty	will exceed drinking water criteria next week
Forecast horizon	How far into the future a forecast is issued	A forecast of stream discharge one week into the future (a one-week horizon) vs. one day into the future (a one-day horizon)
Forecast skill	The ability of a forecast to accurately predict real world conditions	A forecast that predicts water temperature one week into the future with an RMSE of 1.4° C
Hindcast	A prediction of a time period which has already happened with specified uncertainty but using data which was withheld from the model during calibration and validation. Importantly, hindcasts use hindcasted, not observational, driver data to obtain predictions (see Jolliffe & Stephenson, 2012 for further information)	Daily forecasts of dissolved oxygen in 2018 using a model calibrated with data from 2015 – 2017 and archived meteorological forecasts from 2018
Iterative forecast	The process of repeatedly validating forecasts, updating model initial conditions and parameters, and issuing new forecasts as new data become available	A monthly forecast of fish biodiversity that is validated, updated, and re-issued as fish surveys are conducted between forecasts
Kalman filter (also extended or ensemble Kalman filters)	A method for statistically comparing model predictions and new observations to update the initial conditions and parameters of a model while accounting for uncertainty in both model predictions and observations (see Evensen, 2003 for further information)	Using today’s observation of surface water turbidity to correct yesterday’s model prediction of today’s conditions, while accounting for both uncertainty in model predictions and uncertainty in turbidity sensor observations
Operational forecast	A forecast that is actively being updated and	A one day-ahead water temperature forecast that is

	disseminated to end users	published online to inform community members and fishers
Projection	A forecast based on a specific scenario that could or could not include specified uncertainty	A forecast of phytoplankton concentration next week assuming that algaecide will be applied by reservoir managers tomorrow
Uncertainty partitioning (variance decomposition)	Quantification of the uncertainty contribution from different sources (e.g., uncertainty in initial conditions vs. uncertainty in forecasts of model drivers); usually these contributions and their interactions are summed to estimate "total" forecast uncertainty (see Lofton, Brentrup, et al., 2022 for a freshwater example)	Quantifying the contributions of meteorological forecast uncertainty used to drive a model vs. uncertainty in model parameters to forecasts of lake cyanobacterial density
Uncertainty propagation	Quantitatively accounting for increased forecast uncertainty as the forecast progresses further into the future	The 95% predictive interval for tomorrow's forecasted water temperature is 15.1 to 15.8° C, while the 95% predictive interval for water temperature in 10 days is 11.8 to 20.9° C

Table 2: Definitions and examples of terms used during state-of-art review analysis. Definitions of prediction and forecasting modeling approaches are adapted from Lewis et al. (2022). Definitions of methods for incorporating uncertainty into forecasts are adapted from Dietze et al. (2021). References for definitions of forecast assessment metrics are provided in the table.

Prediction and forecasting modeling approaches		
Term	**Definition**	**Example**
Ecosystem simulation model	Explicitly attempts to simulate ecological processes for a physically-based ecosystem and is too complex to solve analytically	A coupled three-dimensional hydrodynamic-water quality model for a lake
Empirical model	Uses correlations or statistical relationships among variables to make predictions but does not explicitly account for time series attributes of the data	Multiple regression
Machine learning model	Uses time series data of predictors and a target variable (predictand) to train an algorithm that predicts the value of the target variable one or more time steps into the future	Artificial neural network model
Process-based model	Explicitly attempts to simulate ecological processes but is not physically-based and/or is simple enough to be solved analytically	Age-structured population model
Time series model	Uses correlations or statistical relationships among variables to make predictions and explicitly accounts for time series attributes of the data such as autocorrelation and trends	Autoregressive integrated moving average (ARIMA) model

Methods of incorporating uncertainty into forecasts		
Term	**Definition**	**Example**
Assimilates	The forecast system iteratively updates uncertainty in initial conditions and model parameters by comparing model predictions to new data as it becomes available	Using an ensemble Kalman filter to update the uncertainty around a phytoplankton growth rate parameter using the most recent observation of lake chlorophyll-a
Data-driven	The forecast system contains the concept of uncertainty and the degree of uncertainty is informed by data	Confidence interval around a fitted multiple regression line that uses nutrient concentrations and water temperature to predict chlorophyll-a concentrations
Presents	The forecast system contains the concept of uncertainty but values are not derived from data	Using different representative concentration pathway (RCP) scenarios as model drivers to predict distribution of an aquatic invasive species in 10 years
Propagates	The forecast system translates uncertainty in inputs into uncertainty in forecasts, and quantifies how this uncertainty increases into the future	Running a model multiple times with different draws from distributions of parameters, driver data, and initial conditions (i.e., an ensemble) to predict dissolved oxygen from 1 – 10 days into the future
Forecast assessment metrics used in analyzed papers		
Term	**Description**	**Reference**
Area under receiver operating characteristic curve (AUC)	For binary classification predictions, the area under the receiver operating characteristic curve (ROC curve; see definition below) falls between 0 – 1; a value of 0.5 indicates a prediction no	(Bradley, 1997)

	better than chance, while values above and below 0.5 indicates predictions better than chance and worse than chance, respectively	
Bias	For continuous deterministic or probabilistic predictions, difference between mean of predictions and mean of observations; a smaller bias is desirable and bias is expressed in the units of the target variable	(Jolliffe & Stephenson, 2012)
Brier score	Assesses the ability of a model to predict an event by comparing the predicted probability of the event to the binary outcome; ranges from 0 – 1 where 0 is a perfect forecast and 1 is the worst possible forecast	(Brier, 1950)
Continuous ranked probability score (CRPS)	For continuous probabilistic predictions, the ensemble analogue of mean absolute error (MAE; see below); a smaller CRPS is desirable and CRPS is expressed in the units of the target variable	(Gneiting & Raftery, 2007; Matheson & Winkler, 1976)
Mean absolute error (MAE)	The average difference between paired continuous observations and predictions; a smaller MAE is desirable and MAE is expressed in the units of the target variable	(Chai & Draxler, 2014)
Coefficient of determination (R^2)	The proportion of variation in data explained by a model; ranges from 0 – 1 and a higher value of R^2 is desirable	(Nagelkerke, 1991)
Reliability diagram	For continuous probabilistic predictions, a plot of observed relative frequencies vs.	(Bröcker & Smith, 2007)

	forecasted probabilities, where forecasts that follow the 1:1 line are perfect forecasts; alternatively, reliability can be assessed for a given predictive interval by calculating the percentage of observations that fall within the specified predictive interval (e.g., do 90% of observations fall in the 90% predictive interval?)	
Root mean square error (RMSE)	For continuous predictions, the quadratic mean of differences between predicted and observed values; a smaller RMSE is desirable, and RMSE is expressed in the units of the target variable	(Chai & Draxler, 2014)
Receiver operating characteristic curve (ROC)	For binary classification predictions, plots the rate of true positives vs. the rate of false positives; an ROC curve that follows the 1:1 diagonal line indicates a prediction no better than chance, while above and below the 1:1 line indicates better than chance and worse than chance, respectively	(Swets, 1973)
Sharpness	The concentration of a predictive distribution, where the sharper the distribution, the less spread occurs among ensemble members; smaller sharpness is usually considered desirable *providing* the predictive accuracy of the forecast is sufficient (i.e., a sharp, inaccurate forecast is not a good forecast)	(Gneiting, Balabdaoui, et al., 2005)

Table 3: Accuracy of near-term water quality forecasts as reported in reviewed papers. Accuracy is given as a range spanning the full forecast horizon unless otherwise specified (e.g., a continuous ranked probability score (CRPS) of 0.77 – 1.08 º C for a 1 – 5 day water temperature forecast represents the full range of CRPS reported across the 1, 2, 3, 4, and 5-day forecast horizons). In cases when multiple forecast models were used, accuracy is reported for the focal or best-performing forecast model(s) as identified by the authors (i.e., accuracy of null or baseline models is not reported). In cases when multiple forecast methodologies for a single model were trialed (e.g., multiple forecasts generated with a single model but with different ensemble sizes), accuracy is reported across all methodologies. ≅ is used in cases where values are approximated from figures rather than reported in text or tables. Forecast assessment methods which cannot readily be summarized in table format (e.g., reliability plots, tercile plots) were omitted. CRPS = continuous ranked probability score; RMSE = root mean square error; MAE = mean absolute error; MRE = mean relative error; R^2 = coefficient of determination; CI reliability = percent of observations that fall into the 95% confidence interval; RMSEP = root mean square error in probability; AUC = area under the receiver operating characteristic curve; ROCSS = receiver operating characteristic skill score; RPSS = ranked probability skill score; NSE = Nash-Sutcliffe efficiency.

Forecast variable type	Water quality variable	Paper	Year	Ecosystem	Forecast horizon	Length of forecast assessment period	Forecast accuracy
physical	water temperature (surface)	Ouellet-Proulx, St-Hilaire, et al.	2017	river	1 – 5 days	5 summers (15 June to 15 Sept 2009 – 2014)	CRPS = 0.77 – 1.08 ºC across two rivers Brier score for early warning (18 ºC) ≅ 0.12 – 0.18 Brier score for threshold exceedance (20 ºC) ≅ 0.01 – 0.05
physical	water temperature (surface)	Ouellet-Proulx, Chimi Chiadjeu, et al.	2017	river	1 – 5 days	5 summers (15 June to 15 Sept 2009 – 2014)	CRPS = 0.24 – 0.8 ºC across two rivers Brier score = 0.01 – 0.22 across three temperature thresholds (16 ºC, 18 ºC, 20 ºC)
physical	water temperature (multiple depths)	Thomas et al.	2020	reservoir	1 – 16 days	475 days (28 Aug 2018 – 15 Dec 2019	CRPS = 0.23 – 0.80 ºC averaged across all depths Bias 0.03 – 0.05 ºC averaged across all depths RMSE = 0.44 – 1.4 ºC averaged across all depths CRPS skill score (improvement relative to a baseline or null model, where 0 indicates no improvement, 1 indicates a perfect forecast, and values below 0 indicate worse performance than the null) = -0.07 – 0.39 averaged across all depths CI reliability = 79 – 85% averaged across all depths
physical	water temperature (lake outlet)	Baracchini et al.	2020	lake	3 hr – 4.5 days	2 days (28 June – 30 June 2017)	RMSE = 0.8 ºC during upwelling event
physical	water temperature (multiple depths)	Mercado-Bettin et al.	2021	lake & reservoir	1 – 4 months	23 years (Nov 1993 – Nov 2016)	ROCSS significant (representing forecast ability to predict above normal, normal, or below normal temperatures) for below normal winter surface water temperatures in 1 of 4 study lakes; for above normal spring surface temperatures in 1 lake; for below normal spring surface temperatures in 1 lake; for above and below normal summer surface temperatures in 1 lake; for above or below normal winter bottom temperatures in 2 lakes; for above or below normal spring bottom temperatures in 3 lakes; for above or below normal summer bottom temperatures in 3 lakes; for above or below normal autumn bottom temperatures in 1 lake RPSS significant (representing forecast improvement over climatology null model) for surface waters in winter for 1 of 4 study lakes; in spring for 3 of 4; in summer for none; RPSS not significant for bottom waters in winter; RPSS significant for bottom waters in spring and summer for 1 of 4 lakes

Forecast variable type	Water quality variable	Paper	Year	Ecosystem	Forecast horizon	Length of forecast assessment period	Forecast accuracy
physical	turbidity	Jin et al.	2019	river	4 hr	3 months (28 Jul 2014 – 26 Oct 2014)	RMSE = 0.0024 NTU MAE = 0.0421 NTU MRE = 0.2222 NTU R^2 = 0.9698 NTU
chemical	ammonia-nitrogen	Jin et al.	2019	river	4 hr	3 months (28 Jul 2014 – 26 Oct 2014)	RMSE = 0.0487 mg L^{-1} MAE = 0.1045 mg L^{-1} MRE = 0.1991 mg L^{-1} R^2 = 0.9085 mg L^{-1}
chemical	electroconductivity	Jin et al.	2019	river	4 hr	3 months (28 Jul 2014 – 26 Oct 2014)	RMSE = 0.0068 μS cm^{-1} MAE = 0.0635 μS cm^{-1} MRE = 0.3583 μS cm^{-1} R^2 = 0.9424 μS cm^{-1}
chemical	dissolved oxygen	Peng et al.	2020	lake	0 – 5 days	2 years (2017 – 2018)	bias = 0.008 – 0.022 mg L^{-1} RMSEP skill score (percent improvement over baseline model) ≅ 14 – 37% CRPS skill score (percent improvement over baseline model) ≅ 24 – 44%
chemical	ammonium-nitrogen	Peng et al.	2020	lake	0 – 5 days	2 years (2017 – 2018)	bias = 0.001 – 0.028 mg L^{-1} RMSEP skill score ≅ -3 – 18% CRPS skill score ≅ 3 – 32%
chemical	total phosphorus	Peng et al.	2020	lake	0 – 5 days	2 years (2017 – 2018)	bias = 0.001 – 0.003 mg L^{-1} RMSEP skill score ≅ 48 – 78% CRPS skill score ≅ 51 – 76%
chemical	total nitrogen	Peng et al.	2020	lake	0 – 5 days	2 years (2017 – 2018)	bias = 0.008 – 0.016 mg L^{-1} RMSEP skill score ≅ 6 – 42% CRPS skill score ≅ 8 – 40%
chemical	methane ebullition rate	McClure et al.	2021	reservoir	1 – 2 weeks	5 months (17 June – 7 Nov 2019)	RMSE = 0.48 – 0.53 ln(mg CH4 m^{-2} d^{-1}) NSE = 0.76 – 0.80 ln(mg CH4 m^{-2} d^{-1})

Forecast variable type	Water quality variable	Paper	Year	Ecosystem	Forecast horizon	Length of forecast assessment period	Forecast accuracy
biological	chlorophyll-a (integrated over top 5 – 7 m of water column)	Page et al.	2018	lake	1 – 10 days	2 – 3 years (2008 – 2010 for one study lake and 2008 – 2009 for the other)	RMSE ≅ 2.75 – 18.5 mg m^{-3} across two lakes
biological	probability of microcystin health advisory level exceedance	Liu et al.	2020	lake	1 – 5 days	1 summer (Jul – Oct 2017)	bias (binary) = 0.84 – 1.14 for health advisory levels ranging from 0.3 – 20 µg L^{-1} Pierce skill score = 0.19 – 0.41 for health advisory levels ranging from 0.3 – 20 µg L^{-1} AUC = 0.87 for a health advisory level of 6 µg L^{-1}
biological	algal bloom occurrence	Mu et al.	2021	lake	1 – 7 days	assessed hindcasts generated using 10% of available satellite imagery dataset spanning 2002 – 2018 (where total n = 872 images)	84.3 – 97.7% of modeled pixels with CCI% = 0.5 – 1 for bloom occurrence

Figures

Figure 1: The near-term, iterative forecast cycle as implemented in a real-world setting for an operational forecasting system used by managers, decision-makers, or other end users (modified from Dietze 2017). Freshwater forecast end users (e.g., managers, natural resource decision-makers) are engaged at the beginning of the forecast process (Fig. 1 Step A) and a forecasting team is assembled and coordinated (Fig. 1 Step B). The team will then work to develop the models, infrastructure, and workflows needed to produce forecasts (Fig. 1 Step C), and begin obtaining input and validation data for forecasts (Fig. 1 Step D). Before forecasts are generated, the uncertainty associated with the forecast should be quantified (Fig. 1 Step E), and the most recent observational data can be used to update the model (Fig. 1 Step F). Finally, a forecast is generated (Fig. 1 Step G), disseminated to end users (Fig. 1 Step H), assessed (Fig. 1 Step I), and the cycle begins again by seeking end user feedback to help improve the forecast and forecasting workflow (Fig. 1 Step A).

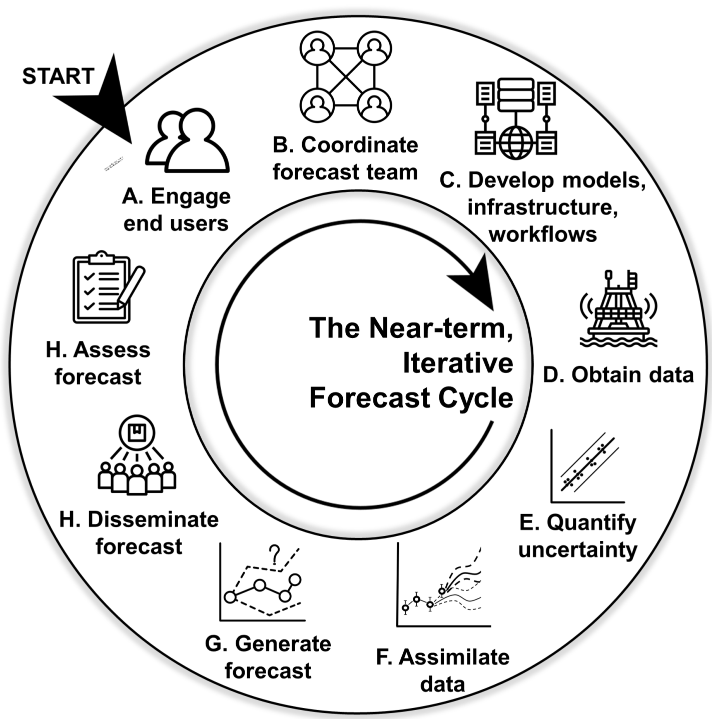


Figure 2: Conceptual framework of our recommendations for advancing the field of freshwater quality forecasting and operational near-term freshwater quality forecasts. Effective forecasts lie at the intersection of freshwater science, end user needs, and relevant tools and skills, all of which require funding support. Agenda items recommended to advance the field of near-term freshwater quality forecasting are in bold, with the italicized number corresponding to sections under "Opportunities to advance near-term freshwater quality forecasting" in the text.

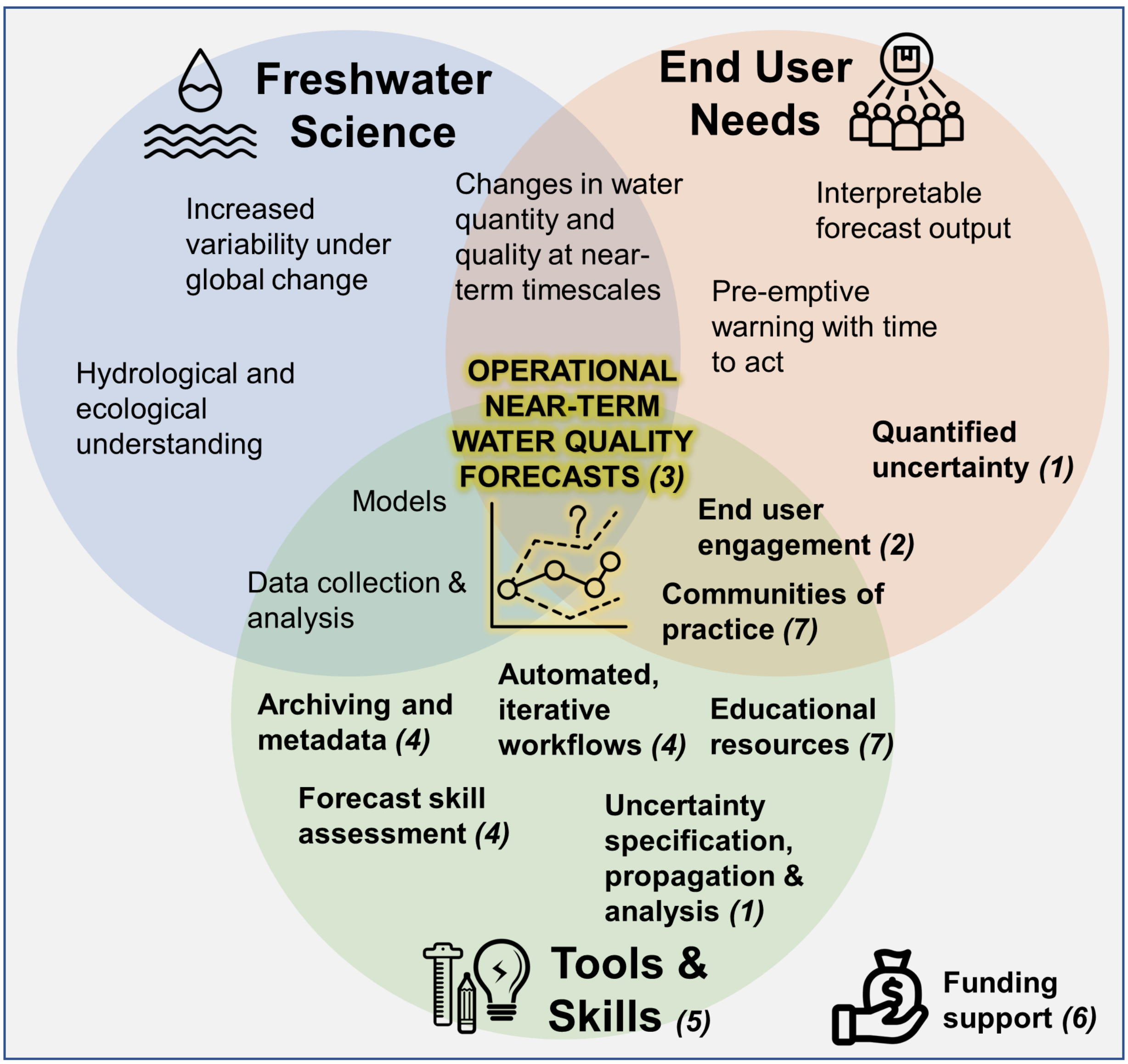


Figure 3: Results of initial screen for state-of-art review. Water quantity is defined as lake or reservoir inflow, stream or river discharge, water level, or flood risk. Near-term is defined as having a minimum forecast horizon ≤ 10 years. Future predictions must have specified uncertainty to be considered a forecast; here, forecast includes forecasts, hindcasts, and projections (see Table 1 for definitions). See Table 2 for definitions of model types, and Fig. S2 for data on model types per category.

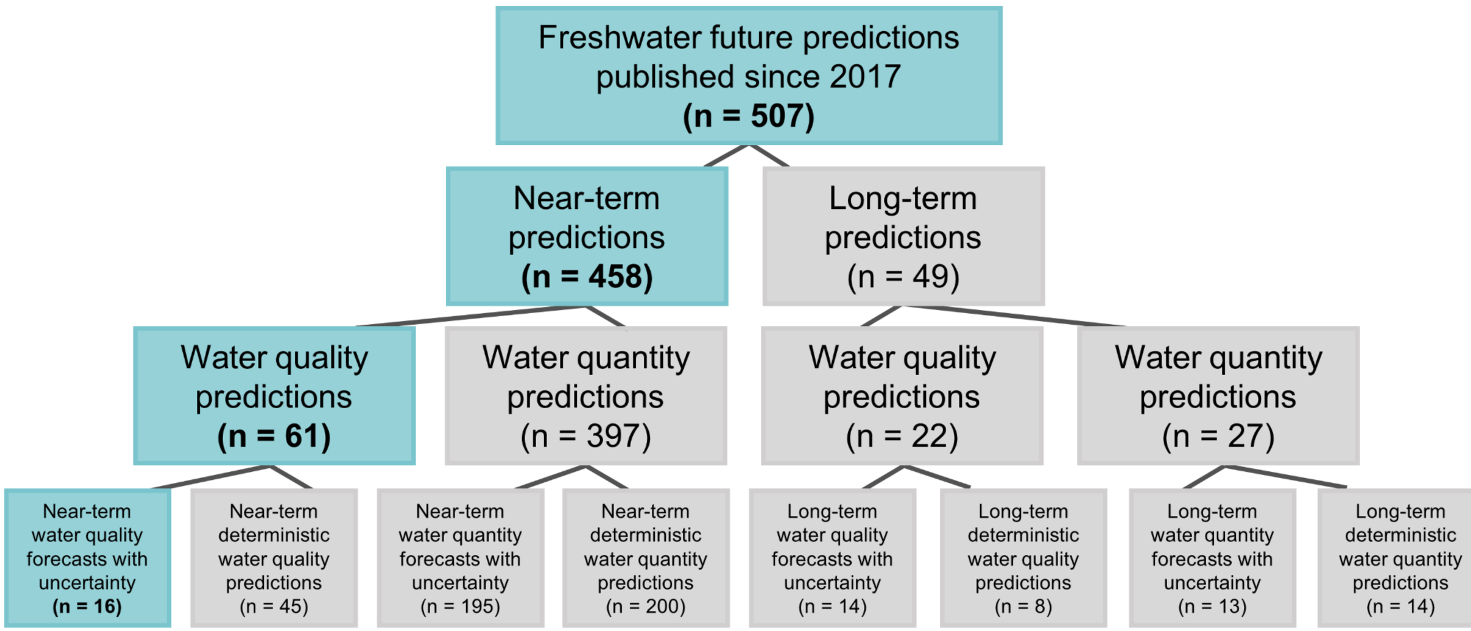


Figure 4: Frequency of water quality variables predicted in papers presenting freshwater future predictions. DO = dissolved oxygen; index = water quality index calculated from multiple freshwater variables; BOD/COD = biochemical oxygen demand/chemical oxygen demand; toxins/T&O compounds = toxins/taste and odor compounds

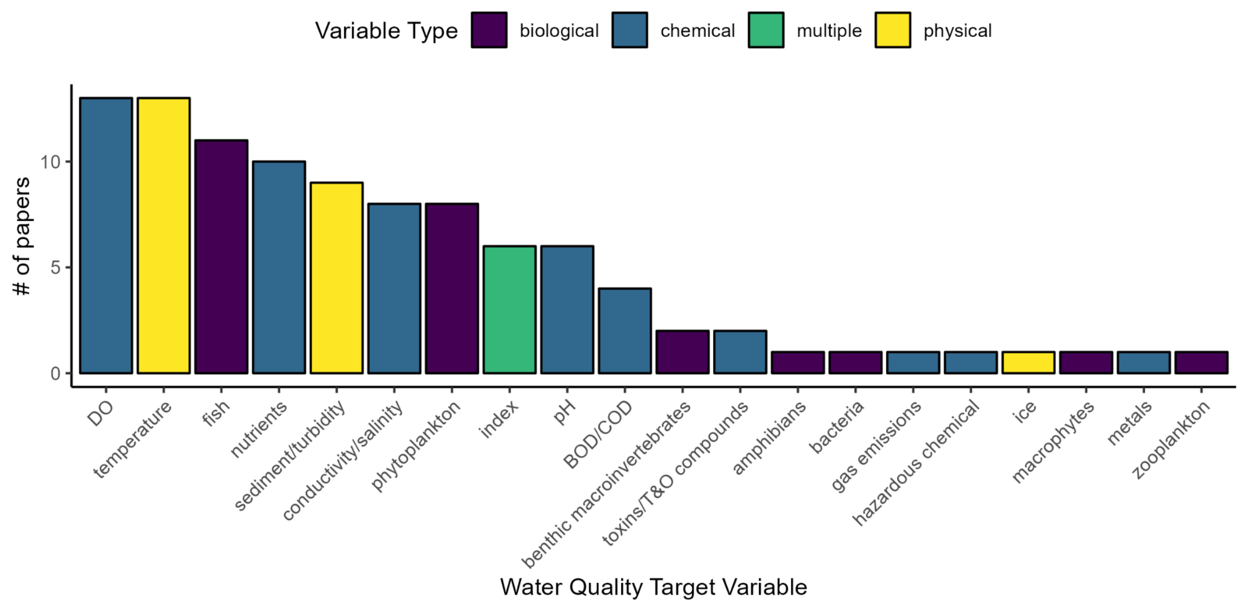


Figure 5: Near-term water quality forecast ecosystem type, target variable type, and maximum forecast horizon. Lentic = standing water (e.g., lake, reservoir); lotic = flowing water (e.g., stream, river). See Table S3 for data underlying this figure.

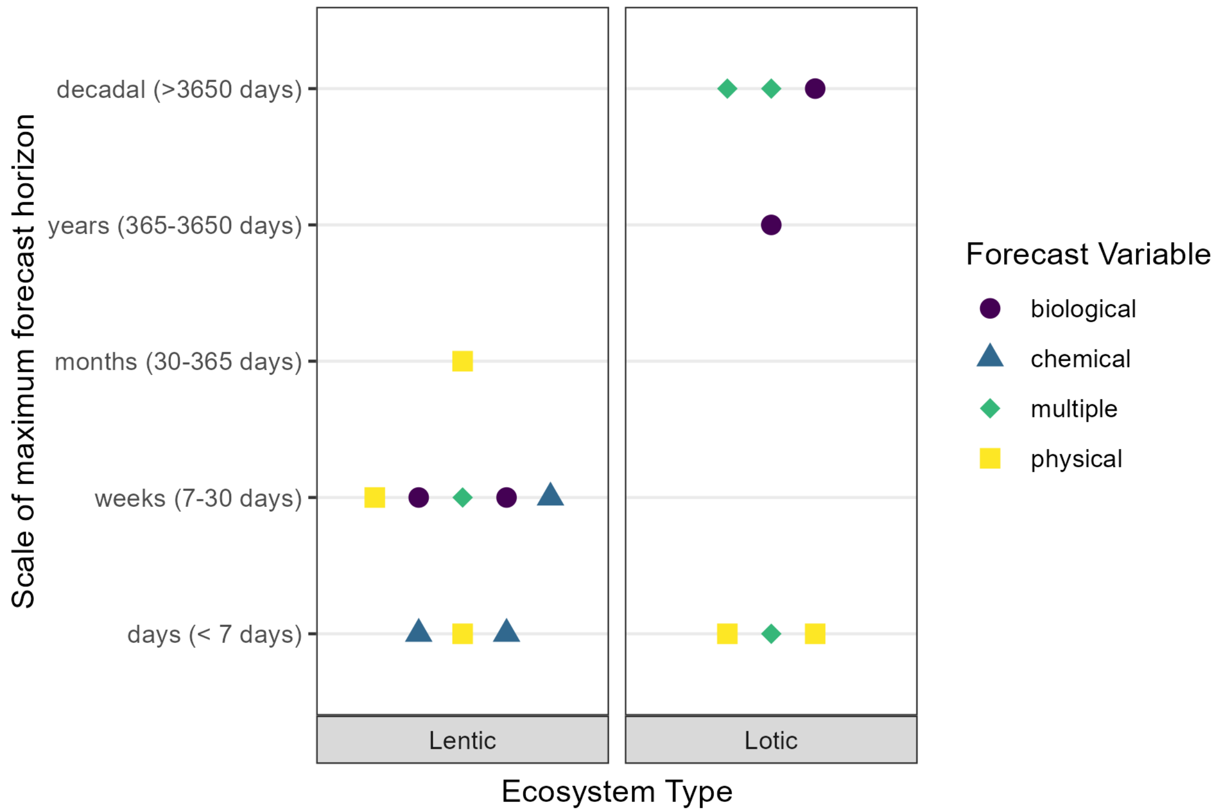
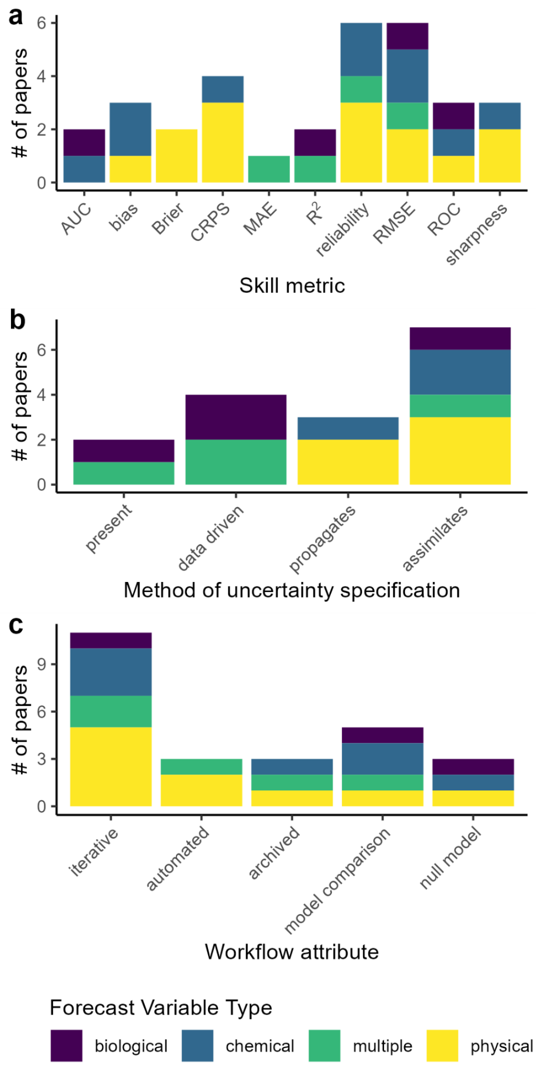


Figure 6: Frequency of a) model calibration, validation, and forecast assessment metrics, b) uncertainty specification methods, and c) workflow attributes for near-term water quality forecasts. See Table 1 for definitions of workflow attributes in (c), Table 2 for definitions of forecast assessment metrics in (a) and uncertainty specification methods (b); and Table S3 for data underlying this figure. AUC = area under receiver operating characteristic curve; Brier = Brier score; CRPS = continuous ranked probability score; MAE = mean average error; R^2 = coefficient of determination; reliability = reliability diagrams; RMSE = root mean square error; ROC = receiver operating characteristic curve.



Supplementary Information for *Progress and opportunities in near-term forecasting of freshwater quality*

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Text S1: *Literature review methods*

Overview

We conducted a state-of-the-art literature review (Grant & Booth 2009) of freshwater forecasting over the past five years to assess the state of the field, recent progress, and ongoing challenges (Fig. S1). First, we conducted a search using the Web of Science^{TM} Core Collection database. Second, we conducted a title screen, followed by an initial full-text screen, during which we assessed whether the paper presented a near-term freshwater quality forecast. Third, we then completed an in-depth analysis of each paper that passed the initial screen using a standardized matrix. Finally, we analyzed the tabular data from our matrix-based paper analysis to assess the state of near-term freshwater quality forecasting and identify areas of recent progress and ongoing challenges. Each step of the literature review process is documented in detail below.

Initial Web of Science search

We built our search around four concepts: forecasting, freshwater, possible freshwater forecast target variables (e.g., streamflow, harmful algal blooms), and a combined global change/resource management concept (Table S1). The final search string required the title to contain a word relating to the forecasting concept and for either the title or the abstract to contain a word or phrase relating to each of the four concepts. After several trial searches, we subsequently removed "predict*" and "project*" from the forecasting concept for the abstract search only, as we found this resulted in retrieval of a large proportion of modeling studies that did not address forecasting. Our search period extended from 1 January 2017 to 17 February

2022, representing the past five years of peer-reviewed research, which is a typical approach for state-of-art reviews (Grant & Booth 2009). Together, these requirements resulted in the following final search string, with the final search conducted on 17 February 2022 yielding 963 results (Fig. S1):

Title must include:

(forecast* OR hindcast* OR predict* OR project*)

Title or abstract must include:

(freshwater OR hydrology OR hydrodynamics OR aquatic OR stream* OR river OR lake OR reservoir OR groundwater) AND (forecast* OR hindcast*) AND (fish OR algae OR phytoplankton OR zooplankton OR plankton OR nitrate OR ammoni* OR nitrogen OR phosphate OR phosphorus OR “dissolved gas” OR “dissolved gasses” OR “dissolved gases” OR “carbon dioxide” OR methane OR nutrient* OR temperature OR communit* OR biodiversity OR flow OR streamflow OR “water quality” OR flood OR hydrology OR hydrodynamics OR “algal bloom” OR “dead zone” OR “dissolved oxygen” OR salmon OR “benthic macroinvertebrate” OR “benthic macroinvertebrates” OR toxin OR cyanobacteria* OR chem* OR biogeochem* OR flux*) AND ((“global change” OR “climate change” OR climate OR “global warming” OR “global cooling” OR “carbon cycle” OR “carbon cycling” OR “greenhouse gas” OR “greenhouse gasses” OR “greenhouse gases” OR hypoxia OR brownification OR “invasive species” OR “land use” OR “nutrient pollution” OR microplastics OR biodiversity OR “emerging diseases” OR antibiotics OR salinization OR eutrophication OR anthrop*) OR (“resource manager” OR “resource management” OR “freshwater resource” OR "freshwater resources" OR "ecosystem service" OR "ecosystem services" OR "water treatment" OR "drinking water" OR "water supply" OR "lake manager" OR "lake management" OR "river management" OR "river manager" OR "water manager" OR "water management" OR "end user" OR "end-user" OR "decision-making" OR "decision support" OR conservation OR "water policy" OR policymaker* OR "water professional" OR "water professionals" OR "water resource" OR "water resources" OR stakeholder* OR research*))

Title and full-text screen

Second, we screened paper titles and text for relevance and basic information regarding forecasts. The title screen was conducted solely by M.E.L. and resulted in elimination of 250 papers, leaving 713 papers for the initial full-text screen (Fig. S1). Examples of papers eliminated during the title screen include papers forecasting vehicular traffic flow and papers forecasting atmospheric rivers, which are a meteorological phenomenon. The initial full-text screen was primarily conducted by M.E.L., with 231 (32%) abstracts double-screened by D.W.H., C.C.C., and R.Q.T. to ensure agreement amongst co-authors regarding interpretation of the screen criteria. The initial screen was conducted using a standardized questionnaire comprising the following questions:

1. Is the study ecosystem an inland waterbody (salty lakes, lagoons, swamps, wetlands are permissible, coastal oceans and estuaries are not permissible)? For studies forecasting runoff or drought/flood risk, there must be some representation of an inland waterbody in the modeling approach.
2. Are the only focal variables some combination of streamflow, inflow, or stream or river discharge, water level or flood risk (i.e., water quantity)?

3. Is the study presenting a forecast, nowcast, or hindcast (defined as a prediction of future conditions from the perspective of the model)?
4. If the study is a forecast, nowcast, or hindcast, is uncertainty specified?
5. If the study is a forecast, nowcast, or hindcast, what modeling approach is used?
6. If the study is a forecast, nowcast, or hindcast, is the forecast/hindcast/nowcast near-term, defined as having a minimum forecast horizon ≤ 10 yr?

In-depth analysis of each paper

Following the initial screen, we conducted an in-depth analysis of all identified near-term freshwater quality forecasting papers (n = 16; Fig. S1) using a standardized matrix (Table S2). Each paper was independently double-screened by M.E.L. and D.W.H., and any discrepancies were resolved through discussion.

Data analysis

Finally, we analyzed our tabular data from both the initial screen of freshwater forecasts and in-depth analysis of near-term freshwater quality forecasts to assess the state of the field of freshwater forecasting as well recent progress and ongoing opportunities following our focal research questions (see main text). All tabular data are available in the Environmental Data Initiative repository (Lofton et al., 2022b) and the analysis code is available in the Zenodo repository (Lofton et al., 2022a).

Table S1: Terms included in final search string on Web of Science™ Core Collection database associated with each of the four core concepts of our search: forecasting, freshwater, possible freshwater forecast target variables (e.g., streamflow, harmful algal blooms), and a combined global change/resource management concept. Asterisks (*) were included after many terms to result in the most inclusive search possible, and search terms with multiple words were quoted to ensure that only results with the entire quoted phrase were returned.

Core concepts for search	**Forecasting**	**Freshwater**	**Freshwater variables**	**Global change & resource management**
Search terms	forecast* hindcast* predict* project*	aquatic freshwater groundwater hydrodynamics hydrology lake river reservoir stream*	algae “algal bloom” ammoni* biodiversity biogeochem* “benthic macroinvertebrate” “benthic macroinvertebrates” “carbon dioxide” chem* communit* cyanobacteria* “dead zone” “dissolved gas” “dissolved gases” “dissolved gasses” “dissolved oxygen” fish flood flow flux* hydrodynamics hydrology methane nitrate nitrogen nutrient* phytoplankton phosphate	anthrop* antibiotics biodiversity brownification “carbon cycle” “carbon cycling” climate “climate change” conservation “drinking water” “decision-making” “decision support” “ecosystem service” “ecosystem services” “emerging diseases” “end-user” “end user” eutrophication “freshwater resource” “freshwater resources” “global change” “global cooling” “global warming” “greenhouse gas” “greenhouse gases” “greenhouse gasses” hypoxia “invasive species” “land use” “lake management”

			phosphorus plankton salmon streamflow temperature toxin “water quality” zooplankton	“lake manager” microplastics “nutrient pollution” policymaker* research* “resource management” “resource manager” “river management” “river manager” salinization stakeholder* “water management” “water manager” “water policy” “water professional” “water professionals” “water resource” “water resources” “water supply” “water treatment”

Table S2: Questions included in standardized matrix analysis of near-term freshwater quality forecasting papers.

Forecast variables, scales, models, and skill
What is the forecast ecosystem? Use the term the authors use in the paper.
Is the forecast targeting a physical, chemical, or biological variable, or some combination of the three?
List the target forecast variable(s), separated by commas (e.g., DOC concentration, streamflow).
What is the minimum forecast horizon in days?
What is the maximum forecast horizon in days?
List the forecast skill metric(s) used, separated by commas (e.g., R^2, RMSE); leave blank if forecast not assessed.
Does the paper include a multi-model (2 or more models) comparison?
Does the paper include a simple null model, defined as either a persistence model, the historical mean (climatology), or a first-order autoregressive model?
How is uncertainty incorporated? See Table 2 for methods of incorporating uncertainty into forecasts.
Forecast infrastructure and workflows
Is the forecast iterative, defined as regularly updated and re-issued when new data become available?
Is the forecast described by the authors as automated, meaning it can be reissued without manual intervention by a human?
Is the forecast archived? Select yes if the archiving is noted in the text, otherwise select no/don't know.
Human dimensions of forecasts
What is the stated motivation for forecast development? Be brief; copy-pasting in quotations is fine but indicate this using quotation marks (" "); leave blank if not stated.
Who is the stated end user? Spell out acronyms; leave blank if there isn't one.
How were end users/stakeholders engaged in development? Be brief; leave blank if not applicable.

Table S3: The n=16 near-term freshwater quality forecasting papers that met our criteria for the in-depth analysis, with a subset of their matrix results. Papers are ordered by publication date; see Lofton et al. (2022b) for complete tabular results. The uncertainty methods are defined in Table 2 in the main text.

Authors	**Year**	**Journal**	**Ecosystem type**	**Forecast variables**	**Min. horizon (days)**	**Max. horizon (days)**	**Uncertainty method**	**Iterative**	**Automated**	**Archived**	**Compared models**	**Used null model**	**End user specified**
Ouellet-Proulx et al.	2017	*WATER*	Lotic	water temperature, discharge	1	5	propagates	x					x
Ouellet-Proulx et al.	2017	*JOURNAL OF HYDROLOGY*	Lotic	water temperature, discharge	1	5	assimilates	x					x
Messager & Olden	2018	*DIVERSITY AND DISTRIBUTIONS*	Lotic	*Faxonius rusticus* (rusty crayfish) occurrence	365	3285	data_driven						
Page et al.	2018	*WATER RESEARCH*	Lentic	phytoplankton community structure	1	10	assimilates	x			x	x	
Bhattacharya & Sanyal	2019	*JOURNAL OF EARTH SYSTEM SCIENCE*	Lotic	discharge, sediment yield	3650	3650	data_driven						
Jin et al.	2019	*ENVIRONMENTAL SCIENCE AND POLLUTION RESEARCH*	Lotic	ammonia-nitrogen, turbidity, electro-conductibility	0.17	0.17	data_driven	x			x		
Fraker et al.	2020	*SCIENCE OF THE TOTAL ENVIRONMENT*	Lotic	fish habitat, fish traits	3650	20075	present						
Thomas et al.	2020	*WATER RESOURCES RESEARCH*	Lentic	water temperature	1	16	assimilates	x	x		x	x	x

Authors	Year	Journal	Ecosystem type	Forecast variables	Min. horizon (days)	Max. horizon (days)	Uncertainty method	Iterative	Automated	Archived	Compared models	Used null model	End user specified
Peng et al.	2020	*WATER RESEARCH*	Lentic	dissolved oxygen, ammonium-nitrogen, total phosphorus, total nitrogen	0	5	propagates	x			x		
Chen et al.	2020	*ENTROPY*	Lotic	water resources vulnerability index	1825	5475	present						
Liu et al.	2020	*ENVIRONMENTAL MODELLING & SOFTWARE*	Lentic	probability of microcystin threshold exceedance	1	5	assimilates	x					x
Baracchini et al.	2020	*WATER RESEARCH*	Lentic	water velocity, water temperature	0.125	4.5	assimilates	x	x	x			x
Mercado-Bettin et al.	2021	*WATER RESEARCH*	Lentic	discharge, water temperature	30	120	propagates	x					
Mu et al.	2021	*ECOLOGICAL INDICATORS*	Lentic	algal bloom occurrence	1	7	data_driven						
McClure et al.	2021	*FRONTIERS IN ENVIRONMENTAL SCIENCE*	Lentic	methane ebullition rate	7	14	assimilates	x		x	x	x	
Carey et al.	2022	*INLAND WATERS*	Lentic	dissolved oxygen, water temperature	1	16	assimilates	x	x	x			x

Figure S1: Freshwater forecasting review workflow. All tabular data are available in the Environmental Data Initiative repository (Lofton et al., 2022b), and all analysis code is available in the Zenodo repository (Lofton et al., 2022a).

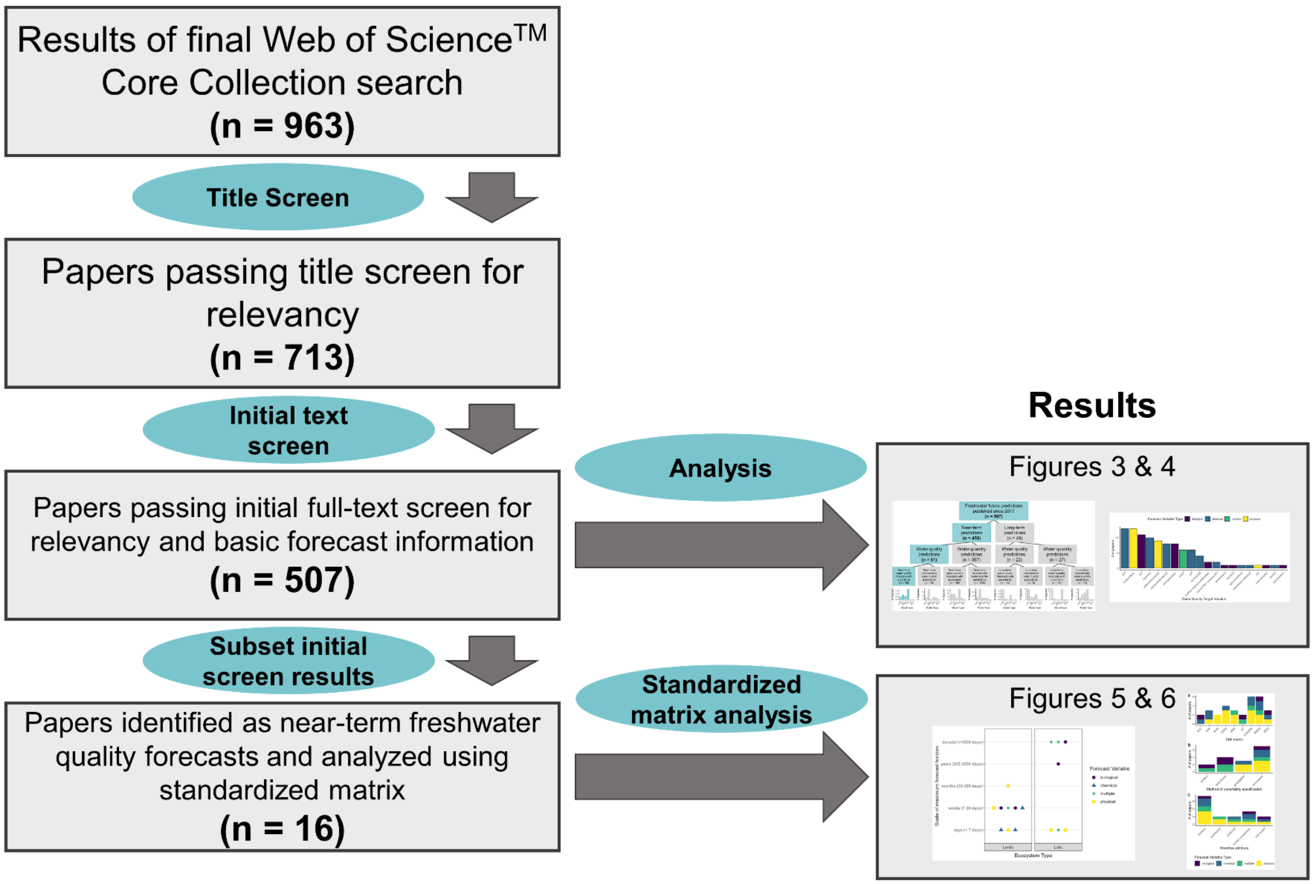
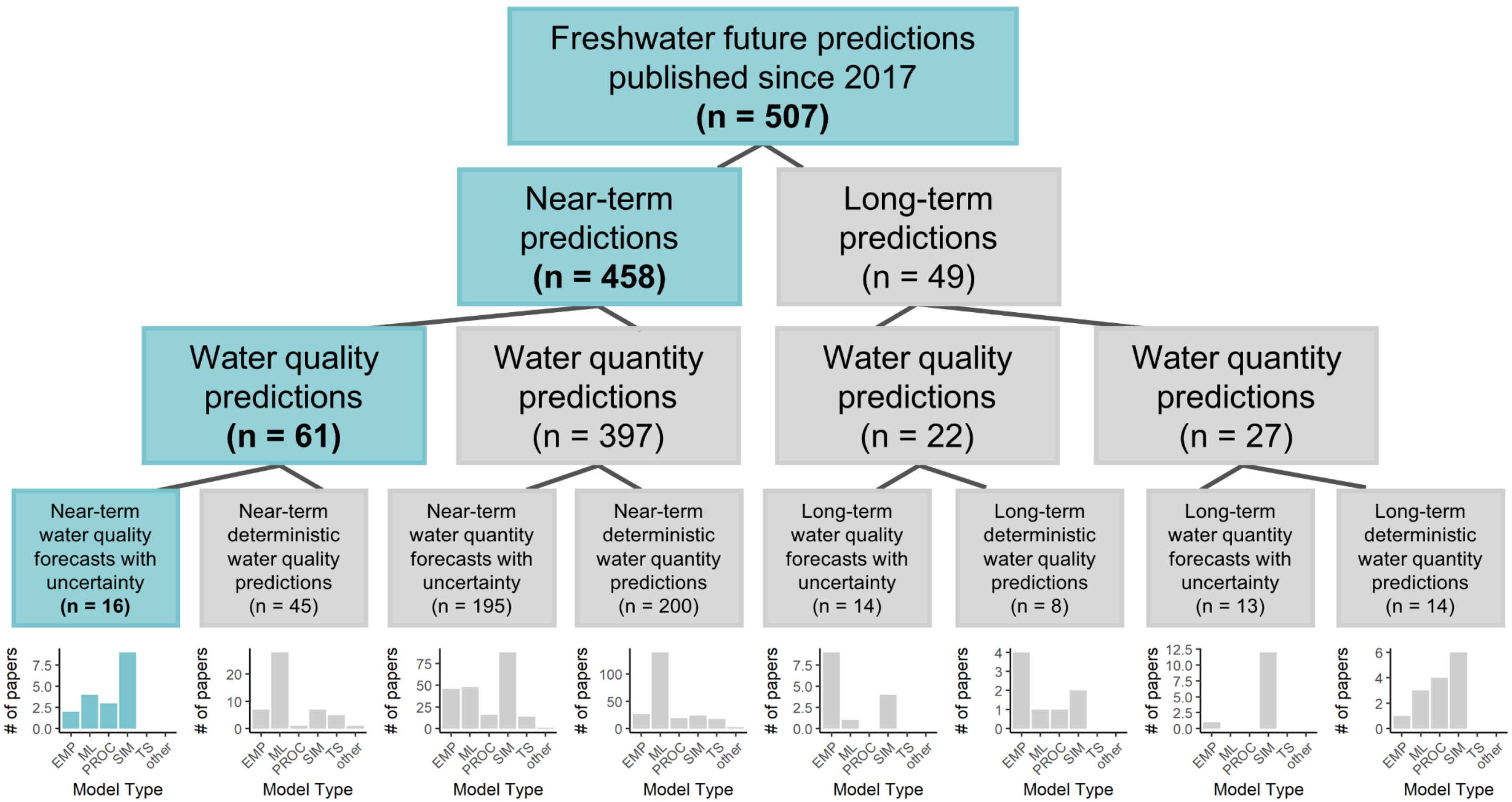


Figure S2: Results of initial screen for state-of-art review. Water quantity is defined as lake or reservoir inflow, stream or river discharge, water level, or flood risk. Near-term is defined as having a minimum forecast horizon ≤ 10 years. Future predictions must specify uncertainty to be considered a forecast; here, forecast includes forecasts, hindcasts, and projections. EMP = empirical model; ML = machine learning model; PROC = process-based model; SIM = simulation model; TS = timeseries model; other = other model type.



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