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

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Contents of this supplement:

Texts: 1

Tables: 3

Figures: 2

Pages: 13

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™ 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).

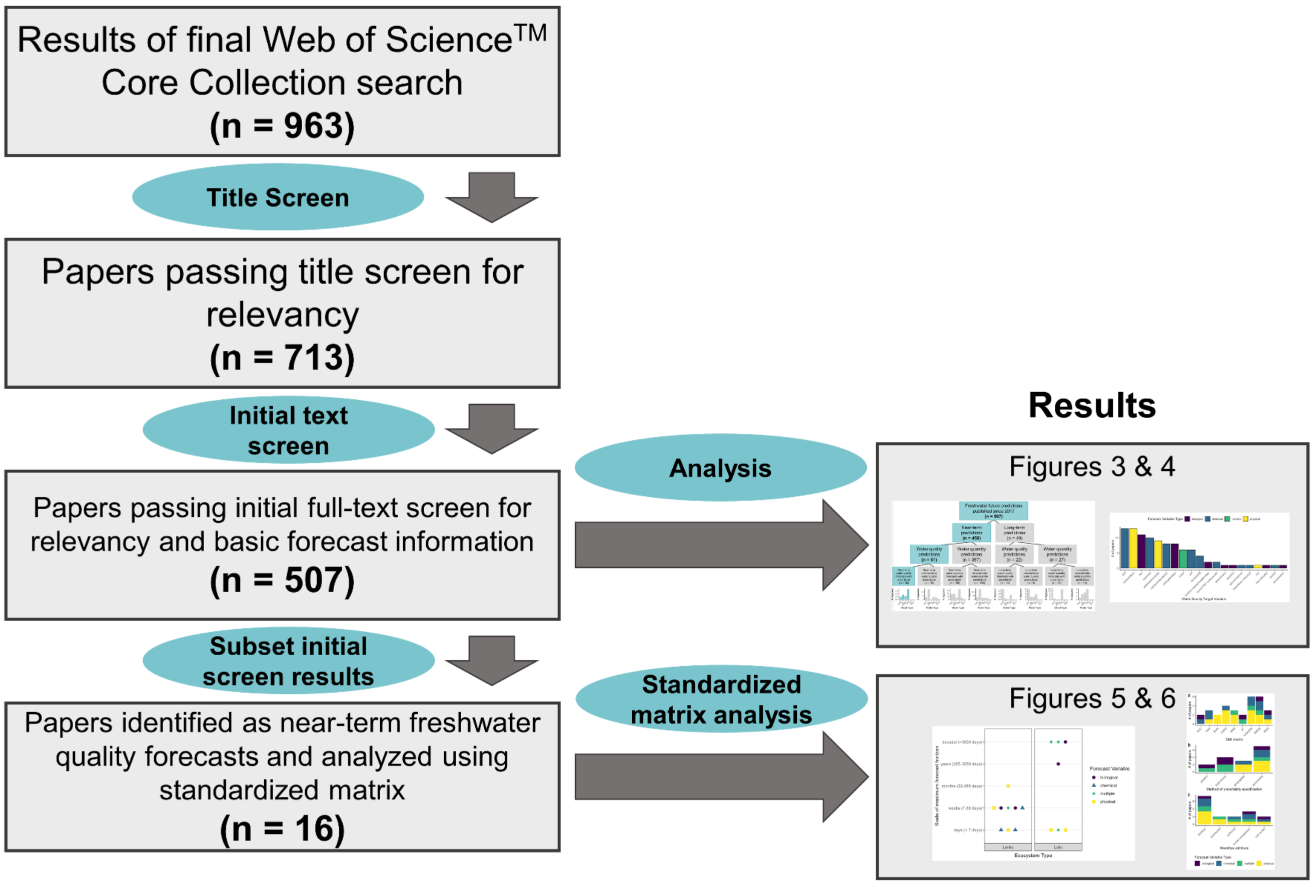
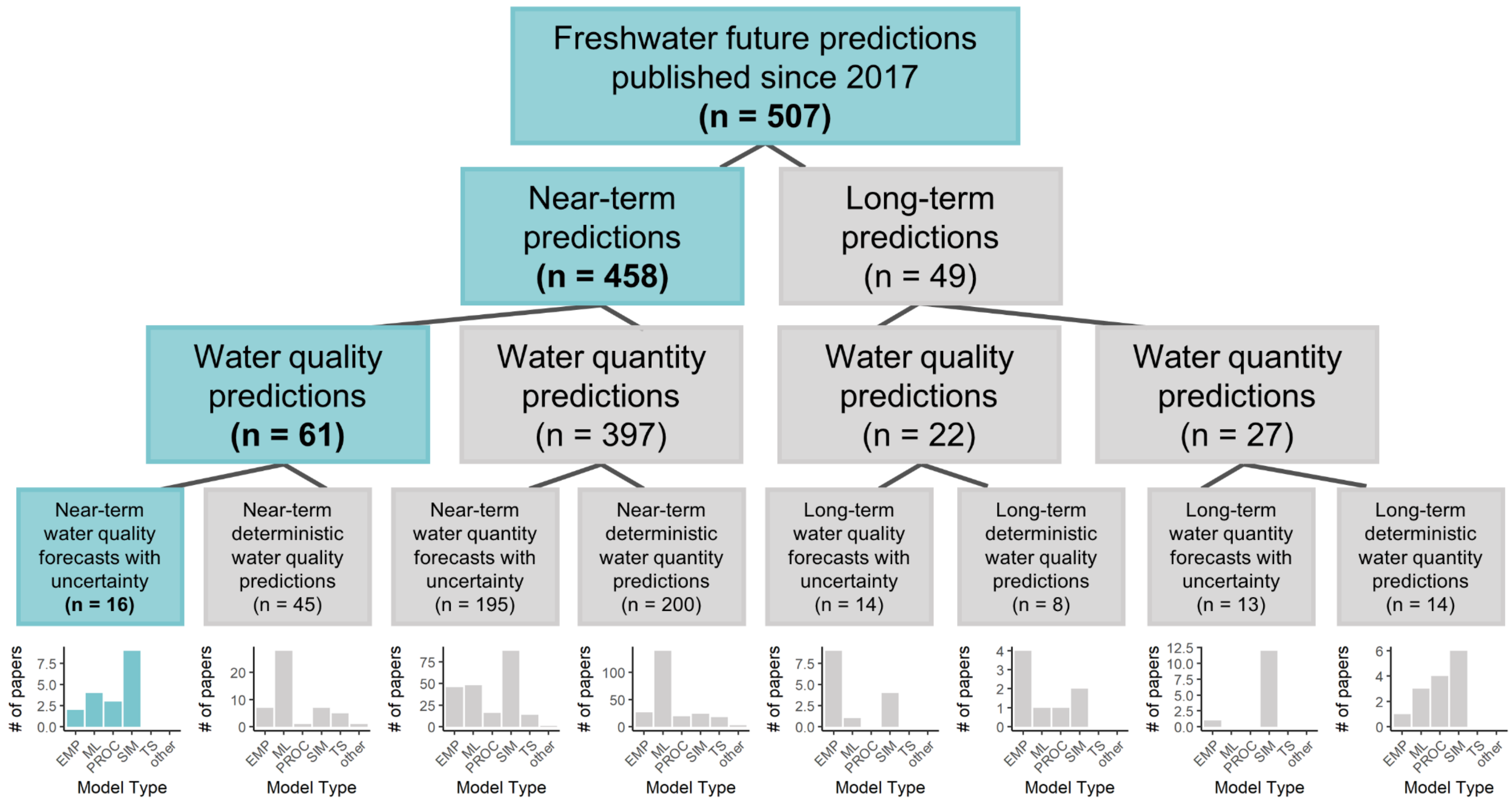


Figure S2: Results of initial screen for state-of-art review. Water quantity is defined as lake or reservoir inflow, stream or river discharge, water level, or flood risk. Near-term is defined as having a minimum forecast horizon ≤ 10 years. Future predictions must specify uncertainty to be considered 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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