

Near-term forecasts of NEON lakes reveal gradients of environmental predictability across the US

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The US National Ecological Observatory Network's (NEON's) standardized monitoring program provides an unprecedented opportunity for comparing the predictability of ecosystems. To harness the power of NEON data for examining environmental predictability, we scaled a near-term, iterative, water temperature forecasting system to all six NEON lakes in the conterminous US. We generated 1-day-ahead to 35-days-ahead forecasts using a process-based hydrodynamic model that was updated with observations as they became available. Among lakes, forecasts were more accurate than a null model up to 35-days-ahead, with an aggregated 1-day-ahead root-mean square error (RMSE) of 0.61°C and a 35-days-ahead RMSE of 2.17°C. Water temperature forecast accuracy was positively associated with lake depth and water clarity, and negatively associated with fetch and catchment size. The results of our analysis suggest that lake characteristics interact with weather to control the predictability of thermal structure. Our work provides some of the first probabilistic forecasts of NEON sites and a framework for examining continental-scale predictability.

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A primary goal of the US National Ecological Observatory Network (NEON) is to “understand and forecast continental-scale environmental change” (NRC 2004). With standardized data available across multiple sites, NEON is uniquely positioned to advance the emerging discipline of near-term, iterative, environmental forecasting (that is, predictions of future environmental conditions and their uncertainty that are updated as additional observations become available) (Dietze *et al.* 2018). However, NEON data have yet to be broadly used for forecasting, a major gap in realizing the potential of the network.

In particular, forecasting the same environmental variables across sites has the potential to reveal gradients of predictability at multiple temporal and spatial scales, a fundamental ecological challenge (Petchey *et al.* 2015; Houlahan *et al.* 2017). Although it has been previously established that forecast accuracy (ie realized predictability) declines with horizon (ie time into the future), how far into the future different ecological variables can be predicted, and how predictability varies among different sites, remain uncertain (Adler *et al.* 2020; Lewis *et al.* 2022). Both site-level (eg lake depth) and

regional-scale (eg weather) characteristics likely affect forecast accuracy at different horizons, but the drivers and gradients of predictability are unknown and may differ among environmental variables.

Lake water temperature is a promising first variable for fulfilling NEON's mission of forecasting environmental change. NEON currently has high-frequency water temperature sensors deployed in six lake sites in the conterminous US, providing a range of water temperature dynamics to forecast. Water temperature is a fundamental property of lakes that governs water chemistry, habitat for biota, and other ecological interactions, yet varies substantially throughout a year as a function of lake morphometry, hydrology, ecology, and weather (Wetzel 2001), making it an ideal forecasting case study. Moreover, forecasts of lake water temperature have practical benefits, as they could help managers choose which depths to extract water for treatment or preemptively apply interventions to mitigate water-quality impairment (Carey *et al.* 2022).

Here, we developed the first known standardized, network-wide forecasts of NEON sites across the US. We applied an open-source forecasting system that uses forecasted weather data and a process-based hydrodynamic model to generate future predictions of lake water temperature for 1-day-ahead to 35-days-ahead. These iterative forecasts were updated with NEON data when they became available. We analyzed the forecasts to address two research questions: (1) how accurately can we predict lake water temperature 1–35 days into the future, and (2) how does forecast accuracy vary among lakes

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with different site-level characteristics and regional-scale weather?

Methods

Forecasting framework

We developed water temperature forecasts for all six NEON lake sites in the conterminous US, which are paired within three NEON-defined ecoclimatic domains (Figure 1). The lakes consisted of two paired lakes in the Great Lakes domain (Crampton Lake, NEON site ID: CRAM; Little Rock Lake, NEON site ID: LIRO), two paired lakes in the Northern Plains domain (Prairie Lake, NEON site ID: PRLA; Prairie Pothole, NEON site ID: PRPO), and two paired lakes in the Southeastern domain (Barco Lake, NEON site ID: BARC; Suggs Lake, NEON site ID: SUGG). The lakes vary in multiple characteristics, including morphometry (depth, volume, surface area, fetch), hydrology (residence time, catchment size), ecology (water clarity), and weather (air temperature, precipitation) (Figure 1; see WebTable 1 for lake metadata). Forecasts were developed for each lake using standardized configurations of Forecasting Lake And Reservoir Ecosystems (FLARE), an open-source forecasting system (Thomas *et al.* 2020; Daneshmand *et al.* 2021). While we previously deployed FLARE on a reservoir in Virginia (Thomas *et al.* 2020) that has similar sensor infrastructure to a NEON site, FLARE had not been deployed on other lakes – until this study.

FLARE forecasts water temperature at multiple depths in the water column using the General Lake Model, an open-source lake hydrodynamic model (Hipsey *et al.* 2019).

FLARE's iterative forecasting cycle can be summarized as follows: (1) each day, the output from the previous day's ensemble forecast (ie a set of equally likely simulations of potential future conditions) is used to initialize an ensemble forecast of the current day's water temperature; (2) FLARE updates the current day's ensemble forecast and key model parameters to be consistent with the current day's observations using data assimilation; and (3) after updating the forecast, a 1 to 35-days-ahead ensemble forecast of the future is generated, for which no observations are yet available for assimilation. We forecasted water temperature at every 0.25–0.5-m depth interval in each of the six lakes, which encompassed all depths with sensors as well as depths without sensors. The forecasts into the future are driven by 1 to 35-days-ahead meteorological forecasts from the National Oceanic and Atmospheric Administration's (NOAA's) Global Ensemble Forecasting System (GEFS) (Hamill *et al.* 2022). We used NEON's water temperature data (Hensley 2022; NEON 2022b,c) for data assimilation and forecast evaluation (WebPanel 1).

An ensemble Kalman filter (EnKF) was employed for data assimilation (Evensen 2009). The EnKF updates model states and parameters based on differences between the ensemble forecast and observations from lake temperature sensors

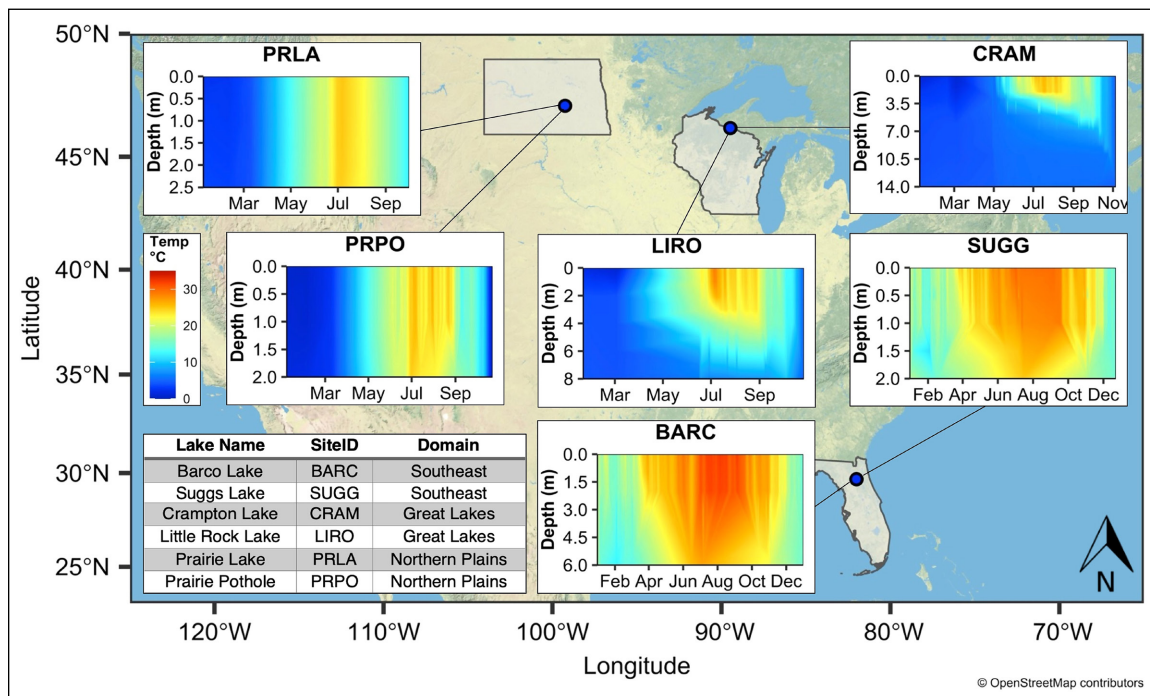


Figure 1. Map showing the locations of the six National Ecological Observatory Network (NEON) lakes forecasted in this study. The inset figures show 1 year of water temperature depth profiles, as measured by automated sensors deployed from a buoy (Hensley 2022; NEON 2022b,c) and monthly handheld probe data collection at each lake (NEON 2022a). The automated sensor data were used in the data assimilation and forecast analysis at depths provided in WebTable 1; the handheld probe data were only used in this figure to better characterize the full water temperature profile. The inset table provides each lake's name, NEON site ID, and NEON ecoclimatic domain. Summary statistics of each lake's morphometry, hydrology, ecology, and weather characteristics are available in WebTable 1. Credit for background map: © OpenStreetMap contributors.

(following Thomas *et al.* 2020). We used this data assimilation approach, rather than directly initiating the forecast with observations, for several reasons. First, data assimilation provided initial conditions for forecasting water temperatures at depths without sensor observations. Second, data assimilation provided initial conditions on days when observations were not available. Third, data assimilation generated initial conditions that combined model predictions and observations based on the relative magnitudes of sensor observation and model error. Finally, data assimilation allowed us to dynamically calibrate the model by updating key model parameters.

Altogether, the ensemble forecasts from FLARE represented uncertainty in initial water temperatures when the forecast was initiated (whereby each ensemble member had a different starting temperature profile set by data assimilation), future meteorology (by associating each ensemble member with a different future weather trajectory from NOAA GEFS), a select set of lake model parameters (whereby each ensemble member was associated with different parameter values set by data assimilation), and lake model equations (whereby normally distributed error representing model process uncertainty was added to each ensemble member at each time-step) (Thomas *et al.* 2020).

Application of FLARE to each lake was initiated on 18 April 2021, the first date when all six lakes had consistent data availability after ice-off. Water temperature data were assimilated but no forecasts were generated from 18 April to 18 May 2021, a spin-up period for initial parameter tuning. Beginning on 18 May 2021, 1 to 35-days-ahead forecasts were produced every day for each lake through 22 October 2021, when data availability ended at the Northern Plains lakes for the year. During the May–October period, data were assimilated and the forecast initial conditions and parameters were updated each day with observations. Other than defining the physical shape of each lake, we performed no lake-specific model calibration, with all lakes sharing the same initial parameters at the beginning of the spin-up period. Data assimilation resulted in a temporally dynamic calibration of the model for each lake. This iterative forecasting cycle resulted in 159 unique 35-day forecasts, each with 200 ensemble members, for each of the six lakes. The results presented below focus on the top 1 m (hereafter, surface).

Evaluation of forecasts

We evaluated forecast performance for each day in the 1–35-day horizon using root-mean square error (RMSE) of the forecasted mean water temperature across ensemble members at each depth and for each horizon (eg the 5-days-ahead RMSE included the 5th day of all forecasts at 1-m depth). Furthermore, we quantified (1) forecast accuracy (defined as RMSE for the first day of the forecast) and (2) accuracy degradation (defined as the difference in maximum and minimum RMSE across the 35-day forecast

horizon). We used Spearman rank correlations to quantify the relationships between lake characteristics (morphometry, hydrology, ecology, and weather) and mean forecast accuracy and accuracy degradation for each lake. We used Spearman rank correlations because the sample size was low ($n = 6$ lakes) and many of the variables were non-normally distributed. To ease interpretation of the correlation coefficient, we negated RMSE so that positive correlations were associated with higher accuracy. Our RMSE calculations only included dates for a given lake when forecasts were available at all 1–35-day horizons.

In addition, forecasts generated by FLARE were also compared to null model forecasts that assumed the forecasted mean water temperature for a date and depth was equal to the mean water temperature observed historically on that day-of-year (DOY). The DOY null model evaluated whether FLARE had higher forecast accuracy than a simple historical mean and was based on all historical NEON data available for a lake (WebTable 1).

Results

Overall, when aggregated across the forecasting period, the forecasts were able to accurately predict surface water temperature within 2.60°C RMSE 1 to 35-days-ahead for all six lakes (Figure 2a; see WebFigure 1 for two example forecasts). The forecasts performed better than a DOY null model at least 35-days-ahead for the Northern Plains domain lakes; at least 30-days-ahead for the Great Lakes domain lakes; and at least 5-days-ahead for the Southeast domain lakes (Figure 2b). The forecasts for surface water temperature in each lake had similar accuracy when aggregating forecasts across all depths with observations (WebFigure 2).

Among all lakes, forecast accuracy decreased as the forecast horizon increased (Figure 2a). At 1-day-ahead, the mean RMSE of all lakes' forecasts was 0.61°C (range across lakes: 0.41–0.90°C); at 7-days-ahead, the mean RMSE of all lakes' forecasts was 1.21°C (range: 0.68–1.55°C); at 21-days-ahead, the mean RMSE of all lakes' forecasts was 2.03°C (range: 1.20–2.45°C); and at 35-days-ahead, the mean RMSE of all lakes' forecasts was 2.17°C (range: 1.14–2.60°C). The decrease in forecast accuracy as the forecast horizon increased was much lower for BARC than the other lakes (Figure 2a). The Southeast and Northern Plains domain lakes exhibited near-linear decreases in forecast accuracy until ~15 to 20-days-ahead, when the declines in accuracy saturated (Figure 2a). In comparison, the Great Lakes domain lakes exhibited a more constant decrease in accuracy throughout the 35-day horizon.

Differences in water temperature forecast accuracy and accuracy degradation among lakes were associated with multiple lake morphometric, hydrological, ecological, and weather characteristics. Although our inference space was extremely limited (with only six lakes), we observed that forecast accuracy was positively correlated with maximum depth and water

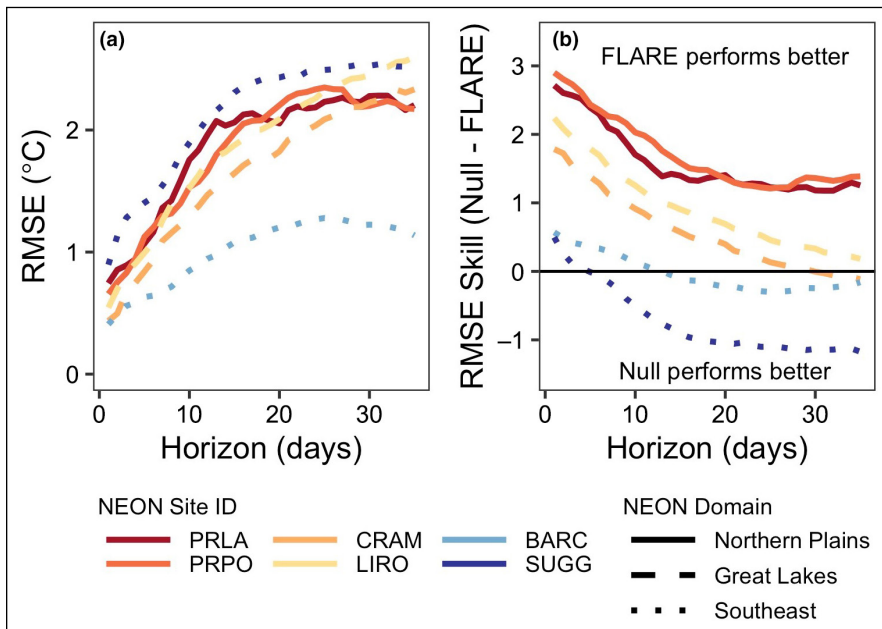


Figure 2. (a) Surface-water temperature (top 1 m) forecast accuracy, defined by the root-mean square error (RMSE, in °C), for 1 to 35-days-ahead (horizon) forecasts at the six NEON lakes. (b) A skill score of the RMSE (in °C) of the null day-of-year model versus forecasts generated by the Forecasting Lake And Reservoir Ecosystems (FLARE) system for each lake. Positive values indicate that FLARE forecasts outperformed the null at a given horizon, zero indicates that the forecasts and null performed similarly, and negative values indicate that the null outperformed the forecasts.

clarity, and negatively correlated with fetch and catchment size (Figure 3; WebTable 2; WebFigure 3). In contrast, accuracy degradation was positively correlated with volume and water clarity, and negatively correlated with mean annual air temperature (Figure 3; WebTable 2; WebFigure 4).

Conclusions

Here, we present the first continental-scale forecasts of lakes uniquely enabled by NEON. We applied the same forecasting framework to six NEON lakes (that is, the hydrodynamic model was configured identically among lakes, all lakes had the same initial model parameters, and each lake received similar amounts of data for assimilation), thereby creating a standardized analysis that can shed light on differences in realized predictability (ie forecast accuracy) among sites. Overall, our forecasts had high accuracy among lakes, with consistent patterns in degradation of forecast accuracy with horizon. Below, we explore gradients in accuracy observed among lakes, as well as how our study provides a framework for future NEON forecasting efforts.

Among lakes, water temperature forecast accuracy was high overall, with a mean 1-day-ahead RMSE of 0.61°C and a mean 35-days-ahead RMSE of 2.17°C. Data assimilation resulted in high accuracy at shorter horizons, with decreased forecast accuracy at longer horizons likely due to degradation in weather forecast accuracy. Regardless of horizon, we witnessed an overall high level of accuracy despite using forecasted, not observed, meteorological

data as model inputs. Our forecast accuracy compares favorably to other multi-lake modeling studies that used observed meteorology as inputs. For instance, Kreakie *et al.* (2021) predicted upper water column temperatures with an RMSE of 1.48°C for lakes across the US with a random forest model. Similarly, Read *et al.* (2014) predicted upper water column temperatures with an RMSE of 1.74°C for Wisconsin lakes with a prior version of the same lake model. By comparing our forecasts to these studies and a DOY null, FLARE's use of automated sensors, data assimilation, and iterative forecasting adds substantial predictive power, especially for the northern lakes, where the forecasts all beat the null model >27-days-ahead.

Environmental drivers of predictability

The correlation analysis suggests potential relationships between forecast accuracy and environmental drivers that inform future research expanding beyond these six NEON lakes (Figure 3). Lake maximum depth, catchment size, fetch, and water clarity exhibited relationships with forecast accuracy. Deeper lakes have more pronounced thermal stratification and greater resistance to wind-driven mixing (Gorham and Boyce 1989), thereby stabilizing their temperatures and increasing their predictability. In contrast, lakes with larger catchments experience greater inflow volumes (Messenger *et al.* 2016) and lakes with longer fetch have increased wind-driven mixing (Rueda and Schladow 2009), both potentially resulting in more variable water temperatures and consequently lower predictability. We observed a positive relationship between forecast accuracy and water clarity, as highlighted in the contrast between the two Southeast lakes, with BARC having approximately 10× higher water clarity than SUGG, and much higher forecast accuracy (Figure 2a; WebTable 1). Deeper penetration of solar radiation results in more uniform heating of surface waters, thereby increasing deep-water temperatures and decreasing vertical temperature gradients (Kirillin and Shatwell 2016). Altogether, the higher predictability of water temperature in BARC than SUGG may be due to the interacting drivers of greater depth, smaller fetch, and greater clarity, as well as other factors.

Forecast accuracy degradation was negatively related to mean annual temperature and positively related to water clarity and volume. The colder northern lakes (Northern Plains and Great Lakes domains) exhibited much greater degradation than one of the warmer Southeast lakes (BARC) (Figure 2a), potentially driving the relationship between air temperature and forecast degradation. While the two lakes with the highest water clarity (CRAM and LIRO in the Great Lakes domain) experienced a greater decline in forecast accuracy over the

35-day horizon than the three lakes with the lowest water clarity (PRLA, PRPO, and SUGG), therefore driving the correlation, BARC was an important outlier because it had the highest water clarity yet the lowest decline in forecast accuracy (WebFigure 4). The patterns between degradation and water clarity/volume may have been an artifact of the lakes in the analysis, as the Great Lakes domain lakes had the greatest water clarity and volume and were the only lakes for which forecast accuracy did not saturate with horizon (Figure 2a; WebTable 1). We did not observe strong correlations between forecast accuracy/degradation and the other lake characteristics (Figure 3), although as noted above, our inference space (with six lakes) was limited. However, this initial analysis helps develop hypotheses on the drivers of lake water temperature predictability that can be tested in future work.

Using FLARE to forecast NEON lakes

Our deployment of FLARE to the NEON lakes both extends its current application from one reservoir in Virginia (Thomas *et al.* 2020) to six lakes across the US and increases its maximum forecast horizon from 16 days in the prior application to 35 days. FLARE forecasts of water temperature in the Virginia reservoir had similar accuracy to the forecast accuracy for the lakes in this study (RMSE of 0.52°C at 1-day-ahead and RMSE of 1.62°C at 16-days-ahead, at 1-m depth), and similar degradation of water temperature forecast accuracy with horizon (Thomas *et al.* 2020). Our study also provides further evidence that FLARE can be used to generate accurate forecasts rapidly, with only 1 month of spin-up following spring sensor deployment at the NEON lakes and initiating the spin-up with default model parameters. Notably, we found that water temperature forecast degradation may saturate at longer horizons for some lakes (Figure 2a), which was only made possible by the recently extended duration of the NOAA meteorological forecasts as FLARE inputs.

We note caveats of this work. First, forecast accuracy/degradation is related to the ability of the lake model to simulate water temperature, and as a consequence using a different model may influence the relationships we observed between lake characteristics and accuracy/degradation (Figure 3). Second, our DOY null model was limited to <4 years of data, depending on site (WebTable 1). As additional data become available, this null model will potentially become more accurate, and may outcompete the forecasts at additional horizons.

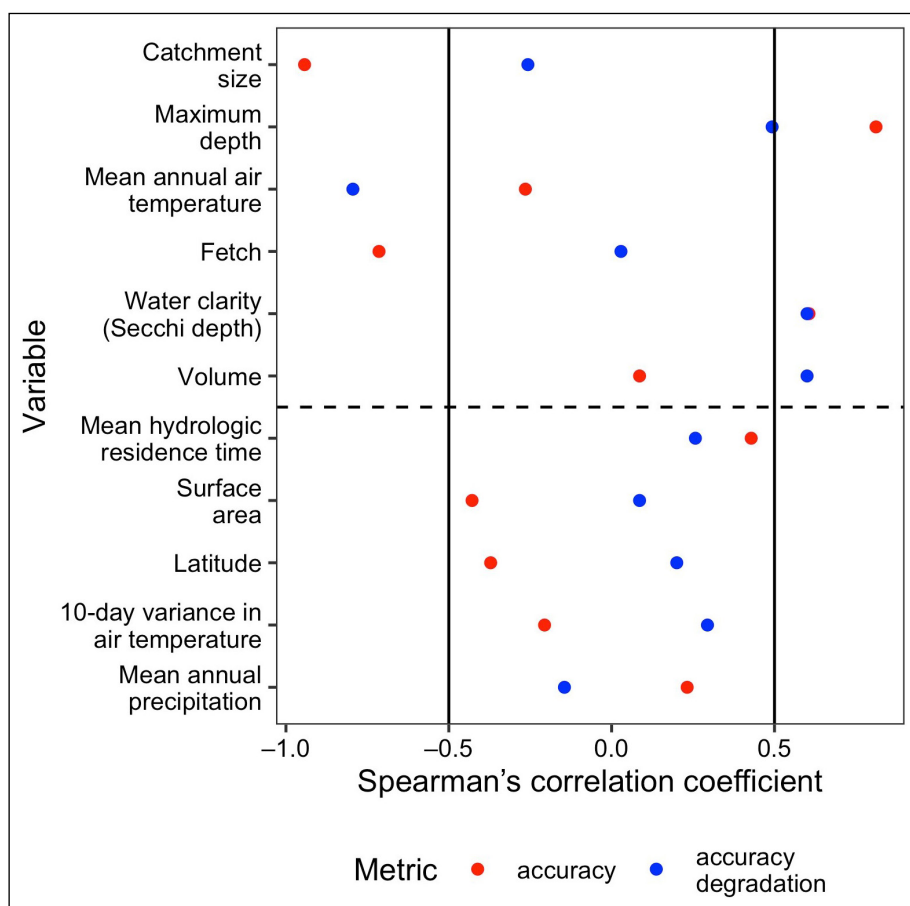


Figure 3. Spearman correlations between two metrics defining predictability at the six lakes: forecast accuracy (red circles), defined as RMSE at 1-day-ahead, and forecast accuracy degradation (blue circles), defined as the difference in maximum and minimum RMSE across the 35-day forecast horizon. For water clarity, note that the symbol of the forecast accuracy metric is obscured by the symbol of the forecast accuracy degradation metric, as the rho values for each metric were identical (0.6). To ease interpretation of the correlation coefficient, we negated RMSE so that positive correlations are associated with higher accuracy. Given the extremely limited sample size of lakes ($n = 6$), which is too small for reliable P values for rho, we focused our interpretation on Spearman rho correlations $|\rho| \geq 0.5$ (above the dashed horizontal line). The relationships are shown as scatterplots in WebFigures 3 and 4.

Third, we only forecasted 1 year of water temperature due to the recent deployment of NEON infrastructure in the study lakes, and our findings may change as we forecast water temperature in future years due to interannual variability. As NEON continues monitoring these lakes into the future (NRC 2004), the hypotheses generated in this initial analysis can be tested. Fourth, the correlation analyses were constrained by small sample size, low variability in characteristics within an ecoclimatic domain (eg the Northern Plains lakes are similar along many axes of potential variation), and collinear variation across domains (eg the deep lakes are only in the Great Lakes domain) (WebTable 1), an inherent limitation of the NEON sampling design. Supplementing future NEON cross-lake forecast comparisons with other lakes (eg those in the Global Lake Ecological Observatory Network) (Weathers *et al.* 2013) would extend key environmental gradients and allow evaluation of whether our observed patterns are

supported by a larger sample of forecasts. This extension is important given that the six conterminous NEON lakes are not representative of the full range of lakes across the US, and the addition of larger and deeper lakes with surface inflows would greatly benefit our analysis.

Power and limitations of NEON for cross-lake forecasting

Similar to weather forecasting – in which increased data availability from sensors and satellites, improved models, and advanced data assimilation techniques enabled a great increase in the number of forecasts and their prediction accuracy (Bauer *et al.* 2015) – we envision that NEON could catalyze a leap in continental-scale environmental forecasting. NEON's standardized measurements, well-documented metadata, and rigorous data quality assurance/quality control provide a critical foundation for forecasting. However, we note that data latency currently limits the ability to generate real-time forecasts. An automated near-term, iterative forecasting system benefits from near-real-time data availability. Given the 2-week to 1.5-month lag in data availability in NEON's current pipeline, our analysis here was based on hindcasts (ie generating forecasts using forecasted drivers to the perspective of the model but for a past date) (Jolliffe and Stephenson 2012). Unless NEON's data latency decreases, forecast analyses such as ours are limited to predicting the past.

Our study provides a framework that can be adapted for additional lakes – as well as terrestrial NEON sites – for forecasting a range of environmental variables and exploring the drivers of predictability. Next steps for this work include forecasting water temperature in future years for the NEON lakes, as well as incorporating forecasts for additional water-quality variables that NEON monitors, such as dissolved oxygen and chlorophyll-*a*. Forecasting additional water-quality variables would greatly expand the utility of the FLARE workflow for informing management, as well as the use of NEON lakes as a multi-region test-bed for developing forecasting methods that can be applied to other waterbodies. Following Dietze and Lynch (2019), the future is bright for forecasting in ecology, in large part due to observatory networks like NEON.

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setup and FLARE configuration. WMW co-developed the code for generating historical weather forecasts with RQT. CB led the development of the *neonstore* package for downloading NEON data and co-developed the code for forecast scoring with RQT. RTH provided lake metadata and assisted with NEON data interpretation. CCC and RQT drafted the manuscript with feedback from all coauthors.

Data Availability Statement

All data analyzed in this manuscript are published and publicly available at Thomas *et al.* (2022a). This submission used novel code, which is provided in Thomas *et al.* (2022b,c). The analysis is executable as a Binder at: <https://mybinder.org/v2/zenodo/10.5281/zenodo.6267616/?urlpath=rstudio>, with Binder instructions available in WebPanel 1.

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