WebPanel 1. Description of the forecasted NEON lakes, overview of the FLARE configuration for each lake, meteorological driver data, mean day-of-year null model, and guide to reproducibility.

NEON Lake temperature data

We generated forecasts for the six NEON lakes in the conterminous USA (WebTable 1). The six forecast sites were two paired lakes in the Great Lakes NEON ecoclimatic 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 siteID – PRLA; Prairie Pothole, NEON siteID - PRPO), and two paired lakes in the Southeastern domain (Barco Lake, NEON siteID – BARC; Suggs Lake, NEON siteID - SUGG). We excluded the seventh NEON lake site (Toolik Lake) since it was not part of a paired NEON set and it has major surface inflows, unlike the other lakes.

Each lake had 5-10 water temperature sensors (Precision Measurement Engineering Inc. T-Chain RS 232/485 thermistors) deployed at various depths in the water column. The first sensor was deployed 0.05 m below the surface, with remaining depths dependent on the total depth of the lake. Generally, sensors were deployed at more frequent intervals within the upper 1.05 m than at deeper depths. These discrete depth water temperature data are available from NEON (NEON 2022a, b), and were accessed using the *neonstore* R package, which creates a "store" of NEON data on a local computer and eases the iterative downloading of additional NEON data without re-downloading data already within the store (Boettiger *et al.* 2021).

All data were filtered using the quality assurance codes provided by NEON. The 30-minute data product was aggregated to the hour and only the 00:00-01:00 UTC hour was used each day for assimilation and evaluation. The NEON (NEON 2022a, b) data were exported using the *neon_export* function in the *neonstore* R package and archived at Thomas and Boettiger (2022). Gaps in NEON's discrete depth water temperature dataset were filled using water temperature data collected by a YSI EXO2 multiparameter sonde as part of NEON's water quality data product (Hensley 2022).

FLARE and GLM configuration

Adapting FLARE to NEON lakes required configuring six unique GLM models with each lake's bathymetry and physical specifications and developing functions to download and process NEON water temperature data. Across all six lakes, we used the same initial default GLM hydrodynamic parameters (Hipsey *et al.* 2019) and tuned the same set of three parameters governing lake water temperature during data assimilation (lw_factor, kw, and sed_mean_temp). Since none of the six NEON lakes have major surface inflows or outflows and prior applications at a reservoir in Virginia showed limited sensitivity of forecast uncertainty to inflows (Thomas *et al.* 2020), we parameterized each lake without inflows or outflows.

We parameterized the process uncertainty in water temperature to be the same across sites and throughout the water column (standard deviation = 0.75°C). This value was based on the findings of Thomas *et al.* (2020), in which FLARE's process uncertainty was estimated across water column depths at a reservoir in Virginia. The process uncertainty was added to each ensemble member and modeled depth at each daily timestep. Since we expect this uncertainty to be correlated with depth (e.g., if the modeled temperature at a certain depth was 1°C warmer than observed, nearby depths should also likely be too warm as well), we included a correlation length that represents an exponential decay of correlations across depths (following Appendix A in Lenartz *et al.* 2007). The decay in correlation results in stronger correlations in water temperature at closer depths than further away depths. This decorrelation length parameter was set to 2 m.

Similarly, observation uncertainty in water temperature data was set to be the same across lakes and depths (standard deviation = 0.1°C), based on the FLARE application in Thomas *et al.* (2020). Since observation uncertainty represents sensor and sampling uncertainty, we did not expect observation uncertainty to be correlated with depth, and therefore the decorrelation length for this uncertainty source was set to 0 m.

Parameter estimation using the ensemble Kalman filter (EnKF) uses the estimated correlation between parameter values and the size of the errors between the predicted and observed states across ensemble members (Evensen 2009). Ensemble members that require large adjustments in the states to be consistent with observations will also adjust parameters that are correlated with that error. One challenge with estimating parameters using the EnKF is that the variation in parameter values across ensemble members collapses over time. The small variance among ensemble members prevents the parameters from further adjusting to reduce new biases in the model predictions (i.e., the calibration does not change through time).

As a result, parameter estimation methods using the EnKF need to use a technique to prevent a collapse in variance. Here, we use a method called variance inflation, in which the variance in parameter values among the ensemble members is increased at each time-step when data assimilation occurs. The variance inflation increases the spread in the parameters among ensemble members while maintaining the rank order of ensemble members. We used the same variance inflation factor across all parameters and lakes (0.04).

The FLAREr R package that contains FLARE functions can be found in the Zenodo repository (Thomas *et al.* 2022b), as well as the scripts for running FLARE at the six NEON lakes (Thomas *et al.* 2022a). All analyses were conducted in R software version 4.1.1 (R Core Team 2021).

Meteorological inputs

The forecasts were driven by numerical meteorological forecasts produced by NOAA's Global Ensemble Forecasting System (GEFS) version 12 (Li *et al.* 2019). We automated the downloading of ensemble members (n=31 total) from the NOAA GEFS output for each 0.5°×0.5° grid cell that included a NEON lake. NOAA GEFS generates weather forecasts at multiple times per day (00:00, 06:00, 12:00, and 18:00 UTC), which vary in their forecast horizon length (i.e., days into the future). We focused on the GEFS weather forecast that started at 00:00 UTC each day, as 30 of its 31 ensemble members extended 35 days into the future on a 6-hour time step and included all meteorological variables required by the GLM as model driver data. The 6-hour output resolution of each of the 30 ensemble members was temporally disaggregated to 1-hour resolution for use in the GLM following Thomas *et al.* (2020).

We used a "stacked" GEFS product during the 1-month spin-up period. One challenge when using data assimilation to set initial conditions and tune parameters is a potential mismatch between the meteorological data used in the spin-up and data used for generating future forecasts. Since observed and forecasted meteorology are rarely a 1:1 match, a smooth transition from data assimilation to forecasting requires either the forecasted meteorology to be corrected for the site or past meteorological forecasts to be used in place of observed meteorology for data assimilation. Here, we used the latter option because NEON meteorological data has a 1.5-month latency and often has gaps for some of the required meteorological variables. To develop a "stacked" GEFS product, we also downloaded the 0-hour and 6-hour horizon of the forecasts that were initiated every six hours at 06:00, 12:00, and 18:00 UTC each day (the 0-hour and 6-hour for the 00:00 UTC forecast were already downloaded as part of the full 35-day horizon). We then combined the temperature, relative humidity, and wind speed from the 0-hour horizon for all NOAA GEFS forecasts. The flux variables (precipitation, longwave radiation, and shortwave radiation) required using the 6-hour horizon because they integrate the 0^{th} to 6^{th} hour. The 0 and 6-hour horizons were used because they directly follow data assimilation in the GEFS, and therefore are most closely aligned with observed meteorology. The resulting "stacked" product was a 6-hr time-step meteorology product because the time step between the initiation of new forecasts was six hours. The stacked data product was updated each time new GEFS forecasts are available, and thus was near-real time.

To estimate the 10-day variance in air temperature that was used in the predictability correlation analysis, we calculated the running standard deviation over a rolling 10-day window between 18 May 2021 and 31 October 2021 from the "stacked" GEFS product. We used the mean of the 10-day running standard deviation to represent air temperature variance for each lake during the period that forecasts were generated.

All NOAA GEFS 1-hour forecasts and "stacked" products for the six NEON lakes are archived at Thomas et al (2022b).

Mean Day-of-Year Null Forecast

We note that while the 1 to 3.5 years of data at the NEON lakes available for this day-of-year (DOY) null model (see WebTable 1) is a shorter duration than the ~30 years of data typically used in weather forecasting null climatology models, it still included all NEON data available for each lake. Moreover, the DOY null model for the lake with just one year of data (PRLA) performed similarly to the DOY null model for its paired lake (PRPO), which had three years of data (Figure 2b).

Guide to Reproducibility

We have provided all code used to generate forecasts, analyze forecasts, and recreate figures in this manuscript as a GitHub repository that has been archived on Zenodo (Thomas et al. 2022a). There are three steps to the analysis that are documented as separate R scripts within the repository. First, the "01_combined_paper_workflow.R" in the "workflows/neon_lakes_ms/" directory of the repository obtains the NEON data and NOAA GEFS weather forecasts and then runs FLARE on the six sites. Since this script runs 159 separate 35-day horizon forecasts for the six lakes, the time required to generate all forecasts depends on the number and speed of computer processors available and can be a multi-day execution. This first step produces a set of output files for the GLM-based and day-of-year null forecasts in a "forecasts" directory.

Second, each ensemble forecast from the first step is aggregated to a mean with predictive intervals and scored (by matching to the corresponding observation, if available), with the summary statistics and observations saved as a set of scored files (one per output file) in a "scores" directory in the repository. The scoring is generated by the "02_score_forecasts.R" script located in the "workflows/neon_lakes_ms/" directory of the repository. While the scores can be generated using output files from the first step, we also provide the output files as an additional Zenodo repository (Thomas et al. 2022b) that can be downloaded and scored using the script without needing to re-run the forecasts.

Third, the scored files are analyzed using an Rmarkdown script located in the main directory of repository (“analysis_notebook.Rmd“) to produce the figures and data reported in the text. The Rmarkdown script can use the scored files produced by the second step or the scores files available in the additional Zenodo repository (Thomas et al. 2022b).

Our analysis can be reproduced by downloading the Zenodo GitHub repository and running the three scripts associated with the steps described above. Re-running the full analysis requires downloading R, Rstudio, and all the required packages, and as noted above, can take multiple days of execution, depending on the computation available. We provide a script that downloads the required packages (“install.R” in the main directory of the repository). However, there is no guarantee that other versions of R and packages will produce the same results as presented here.

To enable greater reproducibility, we adapted the GitHub repository (Thomas et al. 2022a) to generate a Binder that is produced by mybinder.org (Jupyter et al 2018). Mybinder.org provides a web-based version of Rstudio for re-running our GitHub repository code that uses the same version of R and R packages that we used in this analysis (https://mybinder.org/v2/zenodo/10.5281/zenodo.6267616/?urlpath=rstudio). As a result, there is more confidence that the analysis can be reproduced by harnessing the Binder infrastructure, which directly re-runs the analysis on a remote server and provides an Rstudio interface via a web browser for running the scripts described above for each of the three analysis steps.

There are important caveats to using the Binder. First, at the time of this analysis, mybinder.org is free to use, and therefore its computational resources have limits and processing times can be slow. Consequently, we do not recommend running the full generation of the 35-day forecasts in the Binder. The Binder is ideally suited for exploring the scored forecasts and reproducing the figures and values presented in the text (i.e., the “analysis_notebook.Rmd” script described in the third step above). Second, at the time of this analysis, the Binder does not always consistently launch when accessing the Binder link and occasionally the connection times out. It may require accessing the Binder link again to get a successful launch of the R studio interface.

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WebTable 1. Metadata of the six conterminous U.S. lake sites in the National Ecological Observatory Network. Variables that were included in the predictability correlation analysis included: latitude, maximum lake depth, fetch, volume, surface area, mean Secchi depth, mean annual temperature, mean annual precipitation, variance in air temperature, mean hydrological residence time, and catchment size.

siteID	Lake name	NEON Ecoclimatic domain	Latitude (°N)	Longitude (°E)	Elevation (m)	Maximum lake depth (m)	Fetch (m)	Volume (m^3)	Surface area (km^2)
BARC	Barco Lake	Southeast	29.675982	-82.008414	27	6	425	256888	0.12
SUGG	Suggs Lake	Southeast	29.68778	-82.017745	32	3	867	415356	0.31
CRAM	Crampton Lake	Great Lakes	46.209675	-89.473688	509	19	782	889734	0.26
LIRO	Little Rock Lake	Great Lakes	45.998269	-89.704767	501	10	623	466757	0.19
PRLA	Prairie Lake	Northern Plains	47.15909	-99.11388	565	4	1010	389429	0.23
PRPO	Prairie Pothole	Northern Plains	47.129839	-99.253147	579	4	511	158520	0.11

WebTable 1. Continued

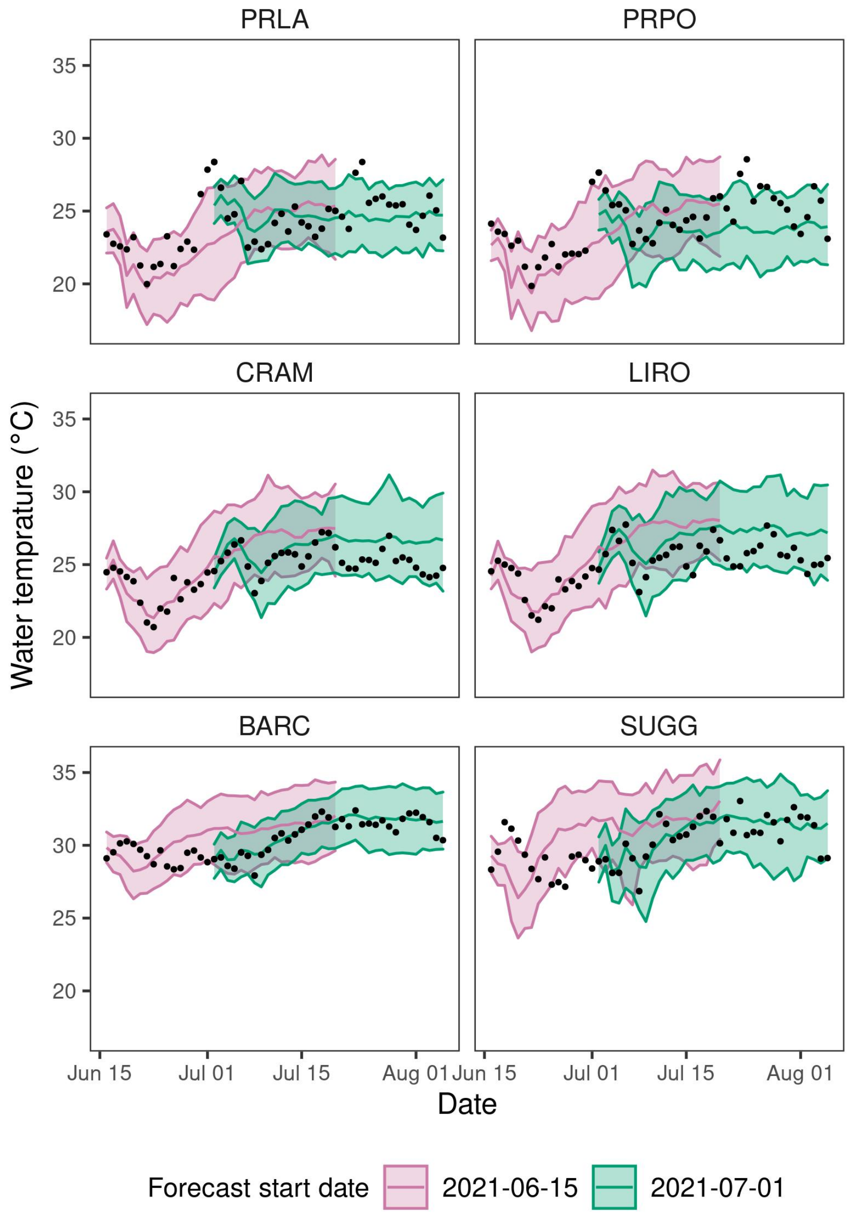
siteID	Mean Secchi depth (m)	Mixing regime	Mean annual temperature (°C)	Mean annual precipitation (mm)	Variance in air temperature (10-day standard deviation, °C)	Mean hydrological residence time (yrs)	Catchment size (km^2)	Number of years in time series for day-of-year null model
BARC	4.08	Polymictic	20.9	1308	1.09	3.3	0.8	2.4
SUGG	0.43	Polymictic	20.9	1308	1.09	1.6	36.9	3.4
CRAM	4.16	Dimictic	4.3	794	2.86	4.9	0.6	2.3
LIRO	4.37	Dimictic	4.4	796	2.86	3.4	0.9	3.1
PRLA	0.33	Polymictic	4.9	490	3.34	3.8	4.5	1.0
PRPO	0.40	Polymictic	4.9	494	3.39	3.2	1.4	2.0

WebTable 1. Continued

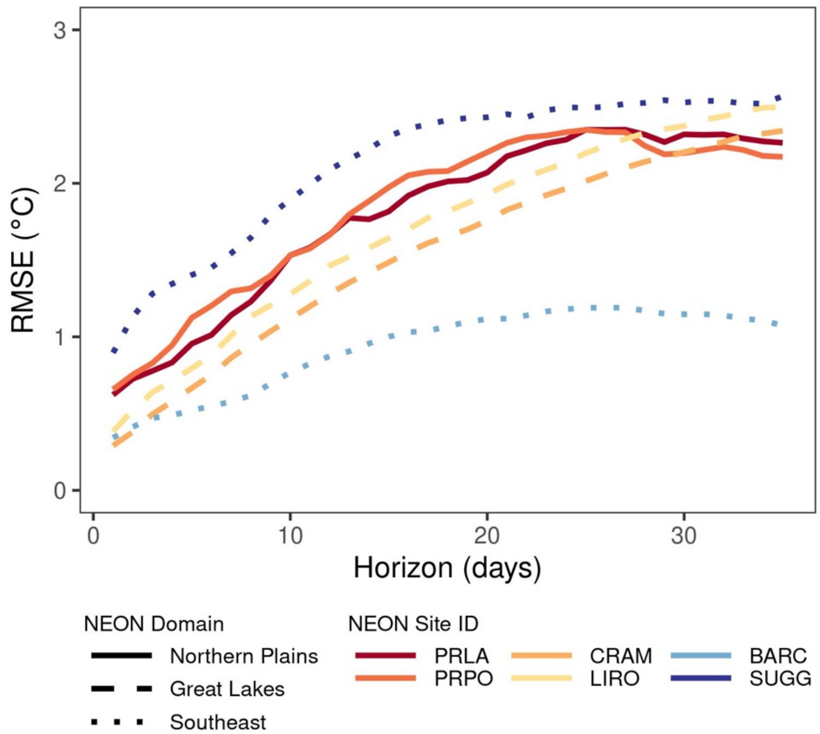
siteID	Catchment land cover	Depths with sensor observations (value is top of 0.25 m thick bin)	NEON Website
BARC	shrub/scrub	0.00, 0.25, 0.50, 0.75, 1.00, 1.25, 1.50, 2.00 2.50, 3.00	https://www.neonscience.org/field-sites/barc
SUGG	evergreen/forest; woody wetlands	0.00, 0.25, 0.50, 0.75, 1.00	https://www.neonscience.org/field-sites/sugg
CRAM	woody wetlands	0.00, 0.25, 0.50, 0.75, 1.00, 1.75, 2.00, 2.50, 3.25, 3.50, 4.25, 4.75, 5.00, 6.25, 6.50, 6.75, 7.75, 8.00, 8.50, 9.25, 9.50, 10.25, 10.75, 11.00 12.00, 12.50, 13.50, 14.00, 15.50	https://www.neonscience.org/field-sites/cram
LIRO	deciduous forest; mixed forest	0.00, 0.25, 0.50, 0.75, 1.00, 1.25, 1.50, 2.00, 2.25, 2.50, 2.75, 3.00, 3.25, 3.50, 4.00, 4.25, 4.50, 4.75, 5.00, 5.75, 6.00, 6.75	https://www.neonscience.org/field-sites/liro
PRLA	grassland/herbaceous	0.00, 0.25, 0.50, 0.75, 1.00, 1.25, 1.50, 1.75, 2.00	https://www.neonscience.org/field-sites/prla
PRPO	grassland/herbaceous	0.00, 0.25, 0.50, 0.75, 1.00	https://www.neonscience.org/field-sites/prpo

WebTable 2. Forecast accuracy, defined as root-mean square error (RMSE) at 1-day ahead, and forecast 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 morphometric, hydrological, ecological, and meteorological characteristics and mean forecast accuracy and accuracy degradation for each lake. To ease interpretation of the correlation coefficient, we negated RMSE so 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 |≥| 0.5 (included here).

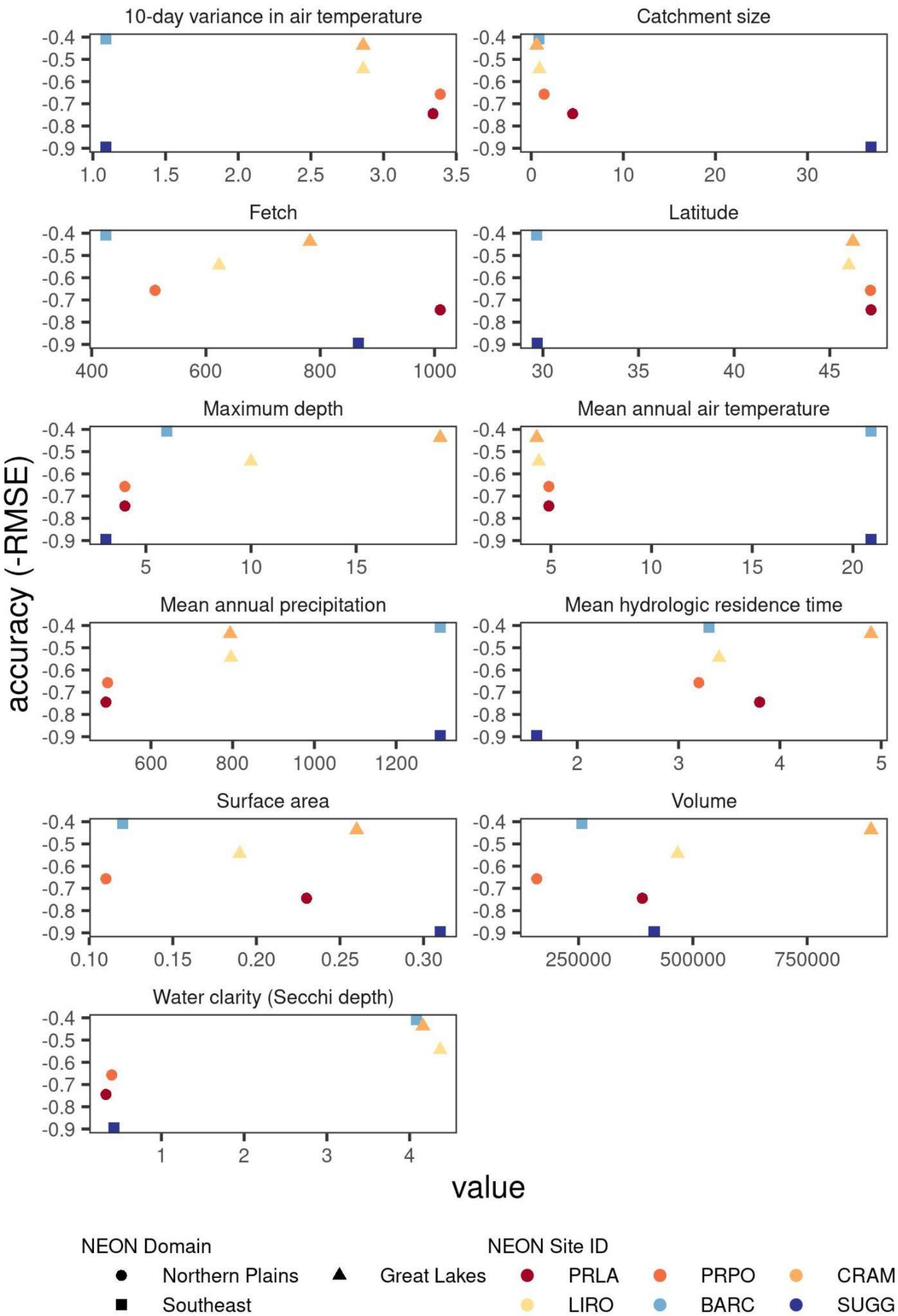
variable	metric	rho
Catchment size	accuracy	-0.94
Fetch	accuracy	-0.71
Maximum depth	accuracy	0.81
Water clarity (Secchi depth)	accuracy	0.60
Mean annual air temperature	degradation	-0.79
Water clarity (Secchi depth)	degradation	0.60
Volume	degradation	0.60



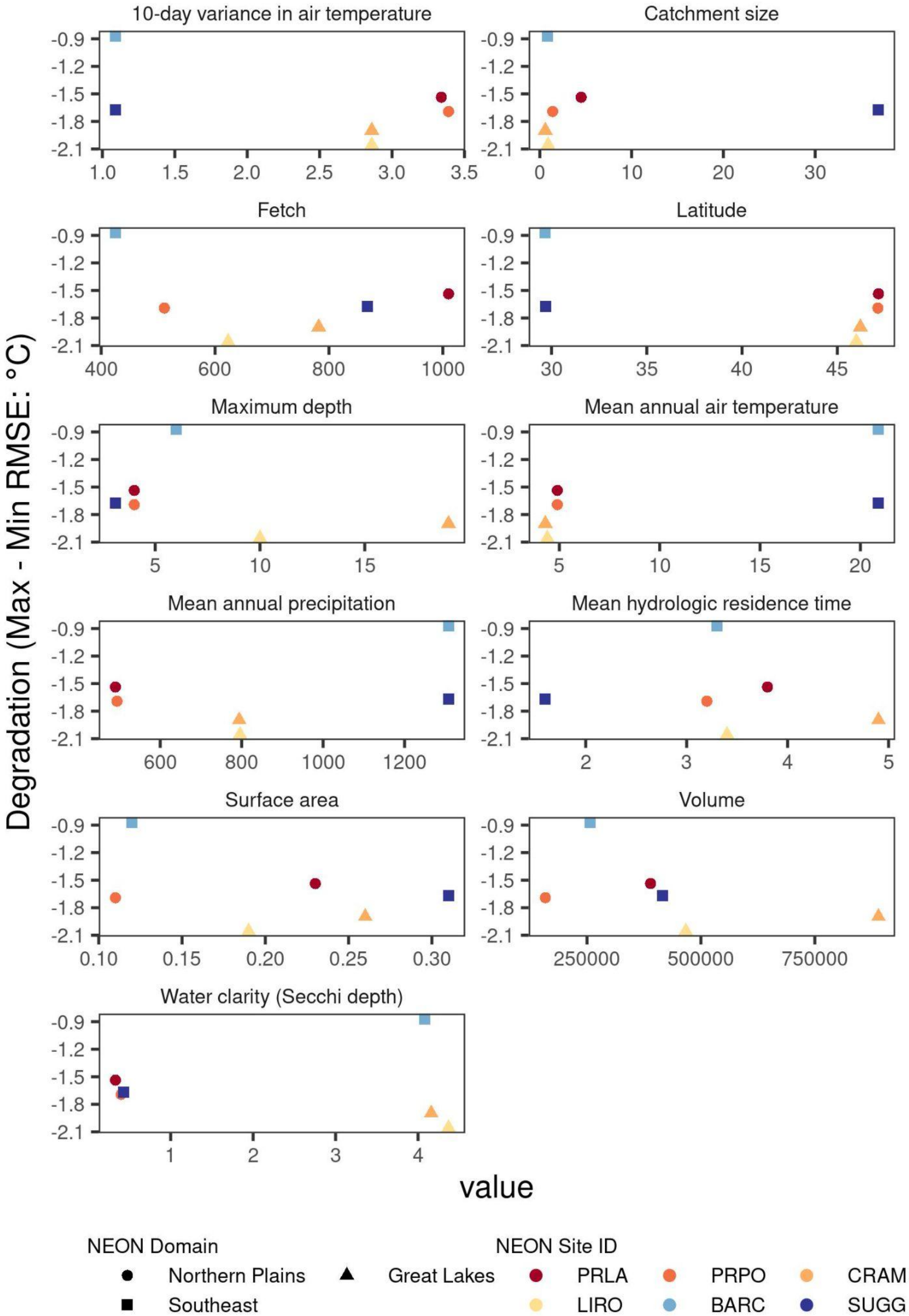
WebFigure 1. Example 35-day forecasts of surface water temperature that were initiated on 2021-06-15 and 2021-07-01. The shaded region represents the 10% and 90% quantiles. The observations (black dots) are provided for reference.



WebFigure 2. Forecast accuracy for water temperature at all depths in each lake aggregated together. Accuracy is defined by RMSE (root-mean square error in °C), calculated separately for each 1 to 35-days ahead (horizon) at the six NEON lakes.



WebFigure 3. Relationships between forecast accuracy (y-axis) and the morphometric, hydrological, ecological, and weather characteristics included in Figure 3 (x-axis). We negated RMSE (root-mean square error in ºC), so positive correlations are associated with higher accuracy. WebTable 1 includes the units for each variable.



WebFigure 4. Relationships between forecast accuracy degradation (y-axis) and the morphometric, hydrological, ecological, and weather characteristics included in Figure 3 (x-axis). Degradation is defined as the difference in RMSE (root-mean square error in ºC) between the maximum and minimum RMSE over the 35-day forecast horizon. WebTable 1 includes the units for each variable.