Near-term forecasts of NEON lakes reveal gradients of environmental predictability across the U.S.

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All data analyzed in this manuscript are published and publicly available at Thomas and Boettiger (2022) and Thomas and Woelmer (2022). This submission uses novel code, which is provided in Thomas *et al*. (2022a) and Thomas *et al*. (2022b). The analysis is executable as a binder at https://mybinder.org/v2/zenodo/10.5281/zenodo.6267617/?urlpath=rstudio

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Abstract

The National Ecological Observatory Network (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 six NEON lakes. We generated 1 to 35-day ahead forecasts using a process-based hydrodynamic model that was updated with observations as they became available. Forecasts were more accurate than a null model up to 35-days ahead among lakes, with an aggregated 1-day ahead RMSE (root-mean square error) of 0.60℃ and 35-days ahead RMSE of 2.17℃. Water temperature forecast accuracy was positively associated with lake depth and water clarity, and negatively associated with catchment size and fetch. Our results 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.

Introduction

A primary goal of the National Ecological Observatory Network (NEON) is to "understand and forecast continental-scale environmental change" (National Research Council, 2004). With standardized data available across multiple sites, NEON is uniquely positioned to advance the emerging discipline of near-term, iterative environmental forecasting – i.e., the prediction of future environmental conditions with specified uncertainty that are updated when observations are 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). While it has been established that forecast accuracy (i.e., realized predictability) declines with horizon (i.e., time into the future), it remains unknown how far into the future different ecological variables can be predicted, and how predictability varies among different sites (Adler *et al.* 2020; Lewis *et al.* 2021). It is likely that both site-level characteristics (e.g., lake depth) and regional-scale characteristics (e.g., weather) affect forecast accuracy at different horizons, but the drivers and gradients of predictability remain unknown and may differ among environmental variables.

Lake water temperature is a promising first forecast 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 U.S., 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, lake water temperature forecasts 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.* 2021).

Here, we developed the first known standardized, network-wide forecasts of NEON sites across the U.S. 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 1-35 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 variability in lake water temperature 1-35 days into the future? and 2) How does forecast accuracy vary among lakes with different site-level characteristics and regional-scale weather?

Methods

Forecasting framework

We developed water temperature forecasts for the six NEON lake sites across three NEON-defined ecoclimatic domains in the conterminous U.S. (Figure 1) using standardized configurations of FLARE (Forecasting Lake And Reservoir Ecosystems), an open-source forecasting system (Thomas *et al.* 2020; Daneshmand *et al.* 2021). 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). FLARE has previously been deployed on a reservoir in Virginia, USA with similar sensor infrastructure to a NEON site but heretofore had not been deployed on other lakes (Thomas *et al.* 2020). FLARE forecasts water temperature at multiple depths in the water column using the General Lake Model (GLM), an open-source hydrodynamic model (Hipsey *et al.* 2019).

FLARE's iterative forecasting cycle is summarized as: 1) each day, the output from the previous day's forecast is used to initialize a forecast of the current day's water temperature; 2) FLARE updates the current day's forecast to be consistent with observations using data assimilation (ensemble Kalman filter; Evensen 2009); and 3) after updating the forecast, a 1 to 35-day-ahead forecast of the future is generated, for which no observations are yet available for assimilation (WebFigure 1). The forecasts into the future were driven by 35-days-ahead meteorological forecasts from NOAA's Global Ensemble Forecasting System (Li *et al.* 2019). Altogether, the ensemble-based forecasts from FLARE included uncertainty in initial water temperatures when the forecast is initiated, future meteorology, GLM parameters, and GLM model equations (Thomas *et al.* 2020). We used NEON's water temperature data (Hensley 2022; NEON 2022a, b) for data assimilation and forecast evaluation (WebPanel 1).

Our application of FLARE for 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–18 May 2021, a spin-up period for initial parameter tuning. Beginning on 18 May 2021, 35-day forecasts were produced every day for each lake through 22 October 2021, when data availability ended at the Northern Plains lakes for the year. This iterative forecasting cycle resulted in 159 unique 35-day forecasts, each with 200 ensemble members, for each of the six lakes. We forecasted water temperature at every sensor depth within a lake: our results below focus on the top 1 m (hereafter, surface) though forecasts for all depths are reported in WebFigure 2.

Evaluation of forecasts

We evaluated forecast performance for each day in the 1–35 day horizon using root-mean square error (RMSE) of the ensemble forecast mean for all depths. 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 morphometric, hydrological, ecological, and weather characteristics and mean forecast accuracy and accuracy degradation for each lake. To ease interpretation of the correlation coefficient, we negated RMSE so positive correlations were associated with higher accuracy. Our analyses only included dates for a given lake when forecasts were available at all 1–35 day horizons.

Additionally, we compared the forecasts generated using FLARE 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 null model evaluated whether FLARE had higher forecast accuracy than a simple historical mean. The DOY null model was based on all available historical NEON data for a lake (WebTable 1).

Results

Overall, aggregated across the forecasting period, the forecasts were able to accurately predict surface water temperature within 2.60℃ RMSE (root-mean square error) 1 to 35 days-ahead for all six lakes (Figure 2a). 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 10 days-ahead for the Southeast lakes (Figure 2b). The forecasts for surface water temperature in each lake had similar accuracy when aggregating forecasts across all depths with observations and when using other evaluation metrics (WebFigure 2).

Forecast accuracy decreased as the forecast horizon increased among all lakes (Figure 2a). At 1 day-ahead, the mean RMSE of all lakes' forecasts was 0.61℃ (range across lakes: 0.41-0.90℃); at 7 days-ahead, the mean RMSE of all lakes' forecasts was 1.21℃ (range: 0.68-1.55℃); at 21 days-ahead, the RMSE of all lakes' forecasts was 2.03℃ (range: 1.20-2.45℃); and at 35 days-ahead, the RMSE of all lakes' forecasts was 2.17℃ (range: 1.14-2.60℃). Forecast accuracy degraded over the 35-day horizon by 41% more in the northern lakes (Northern Plains and Great Lakes domains) than the Southeast domain lakes (Figure 2a). The Southeast and Northern Plains domain lakes exhibited near-linear decreases in forecast accuracy until ~15-20 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 is extremely limited with n=6 lakes, we observed that forecast accuracy was positively correlated to maximum depth and water clarity, and negatively correlated to fetch and catchment size (Figure 3, WebTable 2, WebFigure 3). In contrast, accuracy degradation was positively correlated to volume and water clarity, and negatively correlated to 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 (i.e., the hydrodynamic model was configured identically among lakes, all lakes had the same initial model parameters, each lake received similar amounts of data for assimilation), thus creating a standardized analysis that can shed light on differences in realized predictability (i.e., 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 0.62°C and 35-day-ahead RMSE of 2.21°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 observed 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 example, Kreakie *et al.* (2021) predicted upper water column temperatures with an RMSE of 1.48°C for lakes across the U.S with a random forest model. Similarly, Read *et al.* (2014) predicted upper water column temperatures with an RMSE of 1.74°C for Wisconsin, USA lakes with a prior version of the GLM 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 reveals potential relationships between forecast accuracy and environmental drivers that inform future research. Lake maximum depth, catchment size, fetch, and water clarity exhibited relationships with forecast accuracy. Deeper lakes have stronger thermal stratification and more 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 (Messager *et al.* 2016) and lakes with greater fetch have greater wind-driven mixing (Rueda and Schladow 2009), both potentially resulting in more variable water temperatures and lower predictability. We observed a positive relationship between forecast accuracy and water clarity, as highlighted in the contrast between the two Southeast lakes: Barco had much greater transparency than Suggs, and much higher corresponding forecast accuracy (Figure 2a, WebTable 1). Deeper penetration of solar radiation may result in more uniform heating of the surface waters (following Richardson *et al.* 2017), though this mechanism remains unknown.

Forecast 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 41% greater degradation than the warmer Southeast lakes, likely driving the relationship between air temperature and forecast degradation. The patterns between degradation and water clarity/volume may be 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 correlations between forecast accuracy/degradation and the other lake characteristics (Figure 3), though 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 application 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 USA, as well as increases its maximum forecast horizon from 16 days in the prior application to 35 days. FLARE forecasts of water temperature in the Virginia reservoir have similar accuracy as observed for the lakes in this study (RMSE of 0.52°C at 1 day-ahead and 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). This study also provides more evidence that FLARE can 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. Interestingly, this study reveals 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 GLM to simulate water temperature, so using a different model may influence the relationships we observed between the lake characteristics and accuracy/degradation (Figure 3). Second, our DOY null was limited to <4 years of data, depending on site (WebTable 1). As additional data become available, this null will potentially become more accurate, and may outcompete the forecasts at more horizons. Third, the correlation analyses were constrained by low sample size, low variability in characteristics within an ecoclimatic domain (e.g., the Northern Plains lakes are similar along many axes of potential variation), and collinear variation across domains (e.g., the deep lakes and dimictic 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 (e.g., those in the Global Lake Ecological Observatory Network; Weathers *et al.* 2013) would extend key environmental gradients as well as evaluate whether our observed patterns are supported by a larger sample of forecasts.

Power and limitations of NEON for cross-lake forecasting

Similar to weather forecasting, which exhibited a large increase in the number of forecasts and prediction accuracy after an increase in data availability from sensors and satellites, improved models, and advanced data assimilation techniques (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 QA/QC 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 assumes that data are available in near real-time. Given the 2-week–1.5-month lag in data availability in NEON's current pipeline, our analysis here was based on hindcasts – i.e., 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 adding in forecasts for additional water quality variables that NEON monitors, such as dissolved oxygen and chlorophyll-*a*. 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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Authorship contribution statement

RQT, CCC, and RJF co-developed the FLARE forecasting framework and co-lead the FLARE project. RPM led the development of NEON data processing and FLARE forecasting workflows with assistance from RQT. RPM calibrated lake models with assistance from CCC. TNM assisted with GLM model 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 co-authors. No author has a conflict of interest.

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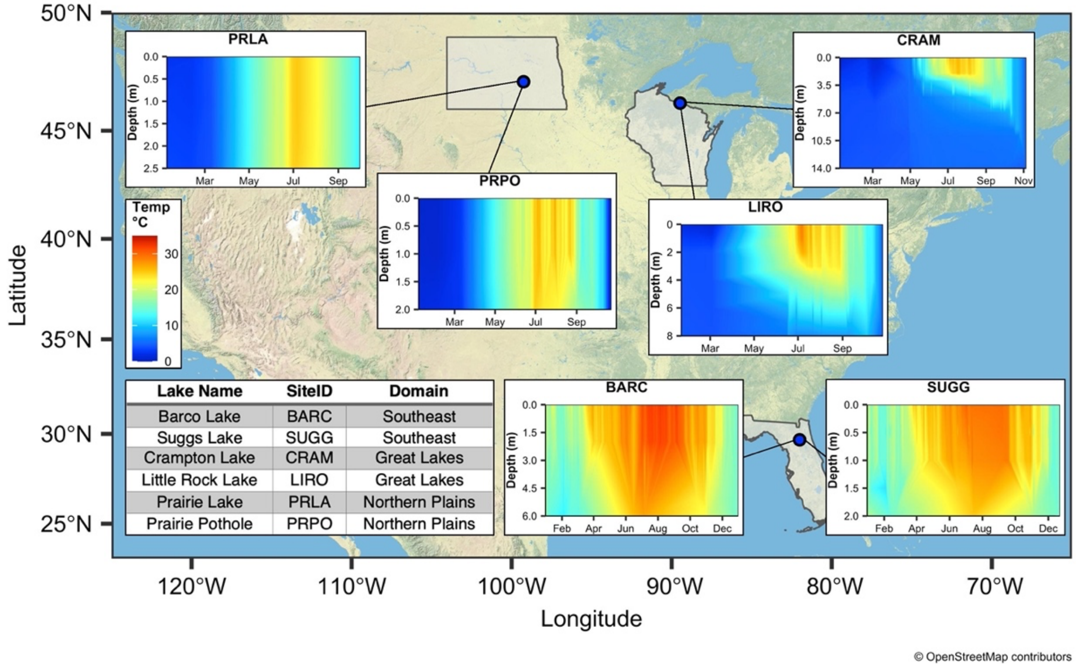
Figure captions

Figure 1. Map showing the locations of the six NEON (National Ecological Observatory Network) lakes forecasted in this study. The inset figures show a year of water temperature depth profiles, as measured by sensors deployed from a buoy at each lake. The inset table provides each lake's NEON Site ID, lake name, and NEON ecoclimatic domain. Summary statistics of each lake's morphometry, hydrology, ecology, and weather characteristics are in WebTable 1.

Figure 2. (a) Surface water temperature (top 1 m) forecast accuracy, defined by RMSE (root-mean square error in ^{o}C), for 1 to 35-day ahead (horizon) forecasts at the six NEON lakes. (b) A skill score of the RMSE (in ^{o}C) of the null day-of-year model vs. forecasts generated by the FLARE (Forecasting Lake And Reservoir Ecosystems) 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.

Figure 3. Spearman correlations between two metrics defining predictability at the six lakes: forecast accuracy (red points), defined as RMSE at 1-day ahead, and forecast accuracy degradation (blue points), defined as the difference in maximum and minimum RMSE across the 35-day forecast horizon. 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 $|\geq|$ 0.5 (above the dashed line). WebFigures 3 and 4 show the relationships as scatterplots.

Figures



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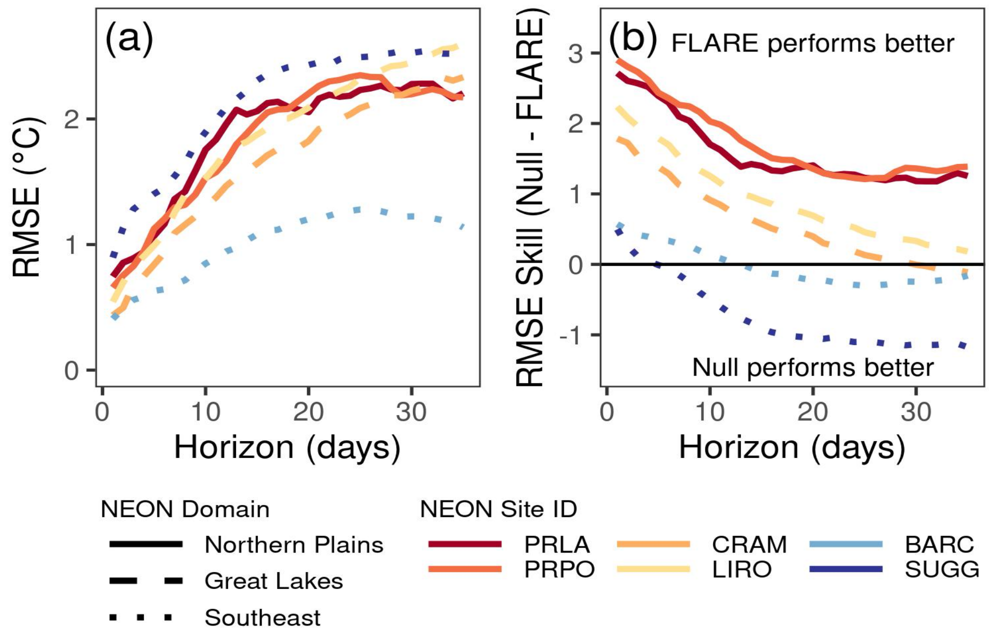

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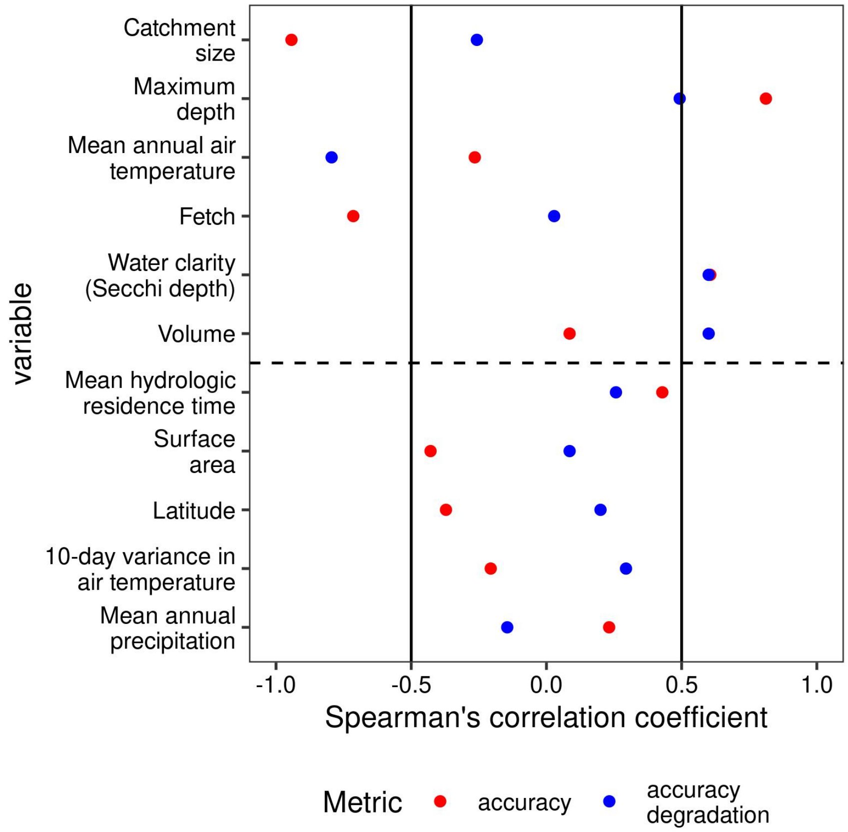

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