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1 %% To submit your paper:  
2 \documentclass[draft,linenumbers]{AGUJournal}  
3 \draftfalse  
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5 %% For final version.  
6 % \documentclass{AGUJournal}  
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8 \journalname{Water Resource Research}  
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10 \begin{document}  
11 \title{A hierarchical model of daily stream temperature for regional predictions}  
12  
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16  
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18  
19 % List up to three key points (at least one is required)  
20 % Key Points summarize the main points and conclusions of the article  
21 % Each must be 100 characters or less with no special characters or punctuation  
22 \begin{keypoints}  
23 \item Flexible approach to modeling daily stream temperature across broad space  
24 \item Allows for inclusion of short observed stream temperature time series  
25 \item Air temperature effects influenced by precipitation and drainage area  
26 \end{keypoints}
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²⁷ **Abstract**

²⁸ Stream temperature is an important exogenous factor influence populations of stream organ-
²⁹ isms such as fish, amphibians, and invertebrates. Given the interest in maintaining cold water
³⁰ fisheries, many states regulate stream protections based on temperature. Therefore, having
³¹ good models of stream temperature is important, particularly for understanding thermal
³² regimes in unsampled space and time. To help meet this need, we developed a hierarchical
³³ model of daily stream temperature and applied it to data from across the eastern United
³⁴ States. Our model accomodates many of the key challenges associated with daily stream
³⁵ temperature models including the non-linear relationship between air and water at very
³⁶ low and very high temperatures, the lagged response of water temperature to changes in
³⁷ air temperature, incomplete and widely varying observed time series, spatial and temporal
³⁸ autocorrelation, and the inclusion of predictors other than air temperature. We used xxxx
³⁹ stream temperature records from xxxx streams to fit our model and xxxx records withheld for
⁴⁰ model validation. Our model had a root mean squared error of xxx for the fitted data and
⁴¹ xxxx for the validation data, indicating excellent fit and good predictive power. We then
⁴² used our model to predict daily stream temperatures from 1980 - 2015 for all streams <200
⁴³ km^2 from Maine to Virginia. From these, we calculated derived stream metrics including
⁴⁴ mean July temperature, mean summer temperature, number of years where the maximum
⁴⁵ daily stream temperature exceeded 20 C, and the thermal sensitivity of each stream reach to
⁴⁶ changes in air temperature. Although generally water temperature follows similar latitudinal
⁴⁷ and altitudinal patterns as air temperature, there are considerable differences at local scales
⁴⁸ based on moderating landscape and land-use factors. We made these metrics available
⁴⁹ through the ecosheds.org web application so that managers and policy makers can use this
⁵⁰ information in natural resource decision making.

51 Introduction

52 Temperature is a critical factor in regulating the physical, chemical, and biological properties
53 of streams. Warming stream temperatures decrease dissolved oxygen, decrease water den-
54 sity, and alter the circulation and stratification patterns of streams (refs). Biogeochemical
55 processes such as nitrogen and carbon cycling are also temperature dependent and affect
56 primary production, decomposition, and eutrophication (refs). Both physical properties and
57 biogeochemical processes influence the suitability for organisms living in and using the stream
58 habitat beyond just primary producers. Additionally, temperature can have direct effects
59 on the biota, especially poikilotherms such as invertebrates, amphibians, and fish [Xu *et al.*,
60 2010b, 2010a; *Al-Chokhachy et al.*, 2013; e.g., Kanno *et al.*, 2013]. Given commercial and
61 recreational interests, there is a large body of literature describing the effects of tempera-
62 ture on fish, particularly the negative effects of warming temperatures on cool-water fishes
63 such as salmonids . Finally, stream temperature can even affect electricity, drinking water,
64 and recreation (see van Vliet *et al* 2011). Therefore, understanding and predicting stream
65 temperatures are important for a multitude of stakeholders.

66 Stream temperature models can be used for explanatory purposes (understanding factors
67 and mechanisms affecting temperature) and for prediction. Predictions can be spatial and
68 temporal including forecasting and hindcasting. Predictions across space are especially
69 valuable because there is often a need for information at locations with little or no observed
70 temperature data. For example, many states have regulations related to the management
71 of streams classified as cold, cool, and warm waters (refs), but because of the tremendous
72 number of headwater streams it is impossible classify most streams based on observed data.
73 Therefore, modeled stream temperature is needed to classify most streams for regulatory
74 purposes. Forecasting can provide immediate information such as the expected temperature
75 the next hour, day, or week as well as long-term information about expected temperatures
76 months, years, and decades in the future. Hindcasting can be used to examine temperature

77 variability and trends over time and for model validation. Both forecasting and hindcasting
78 are useful for understanding climate change effects on stream temperature regimes.

79 Given the importance of temperature in aquatic systems, it is not surprising that there are
80 a variety of models and approaches to understanding and predicting stream temperature.
81 Stream temperature models are generally divided into three categories: deterministic (also
82 called process-based or mechanistic), stochastic, and statistical [Caissie, 2006; Benyahya et
83 al., 2007; Chang and Psaris, 2013]. Deterministic models are based on heat transfer and
84 are often modeled using energy budgets [Caissie, 2006; Benyahya et al., 2007]. The models
85 require large amounts of detailed information on the physical properties of the stream and
86 adjacent landscape as well as hydrology and meteorology. These models are useful for detailed
87 re assessments and scenario testing. However, the data requirements preclude the models
88 from being applied over large spatial extents.

89 Stochastic models attempt to combine pattern (seasonal and spatial trends) with the random
90 deviations to describe and predict environmental data [Kiraly and Janosi, 2002; Sura et al.,
91 2006; Chang and Psaris, 2013]. Stochastic models of stream temperature generally rely on
92 relationships between air and water temperature then with random noise and an autoregressive
93 correlation, often decomposed by seasonal and annual components. These models are mostly
94 commonly used to model daily temperature fluctuations because of their ability to address
95 autocorrelation and approximate the near-random variability in environmental data [Caissie
96 et al., 2001; Kiraly and Janosi, 2002; Ahmadi-Nedushan et al., 2007]. A limitation is that
97 the physical processes driving temperature fluctuations are not elucidated with these models.
98 They are generally used to describe characteristics and patterns in a system and to forecast
99 these patterns in the future [Kiraly and Janosi, 2002]. Additionally, stochastic models rely on
100 continuous, often long, time series from a single or a few locations. Inference cannot be made
101 to other locations without assuming that the patterns and random deviations are identical at
102 those locations.

103 As with stochastic models, statistical models generally rely on correlative relationships
104 between air and water temperatures, but also typically include a variety of other predictor
105 variables such as basin, landscape, and land-use characteristics. Statistical models are often
106 linear with normally distributed error and therefore used at weekly or monthly time steps
107 to avoid problems with temporal autocorrelation at shorter time steps (e.g. daily, hourly,
108 sub-hourly). Parametric, nonlinear regression models have been developed to provide more
109 information regarding mechanisms than traditional statistical models without the detail
110 of physical deterministic models [Mohseni *et al.*, 1998]. Researchers have also developed
111 geospatial regression models that account for spatial autocorrelation within dendritic stream
112 networks [Isaak *et al.*, 2010; Peterson *et al.*, 2010, 2013]. However, due to the complexity of
113 the covariance structure of network geostatistical models, they are best used for modeling
114 single temperature values across space (e.g. summer maximum, July mean, etc.) rather than
115 daily temperatures [Peterson *et al.*, 2007, 2010; Ver Hoef and Peterson, 2010]. Additionally,
116 statistical machine learning techniques such as artificial neural networks have been used to
117 model stream temperatures when unclear interactions, nonlinearities, and spatial relationships
118 are of particular concern [Sivri *et al.*, 2007, 2009; DeWeber and Wagner, 2014b].

119 In contrast with deterministic approaches, statistical models require less detailed site-level
120 data and therefore can be applied over greater spatial extents than process-based models.
121 They also can describe the relationships between additional covariates and stream temperature,
122 which is a limitation of stochastic models. These relationships can be used to understand
123 and predict anthropogenic effects on stream temperature such as timber harvest, impervious
124 development, and water control and release [Webb *et al.*, 2008]. Quantifying the relationship
125 between anthropogenic effects, landscape characteristics, meteorological patterns, and stream
126 temperature allows for prediction to new sites and times using statistical models. This is
127 advantageous for forecasting and hindcasting to predict and understand climate change effects
128 on stream temperatures. This is critical because not all streams respond identically to air
129 temperature changes and the idiosyncratic responses may be predicted based interactions of

₁₃₀ known factors such as flow, precipitation, forest cover, basin topology, impervious surfaces,
₁₃₁ soil characteristics, geology, and impoundments [Webb *et al.*, 2008].

₁₃₂ Letcher et al. [???] outline six general challenges of statistical stream temperature models
₁₃₃ including accounting for 1) the non-linear relationship between air and water temperature at
₁₃₄ high and low air temperatures, 2) different relationships between air and water temperature
₁₃₅ in the spring and fall (hysteresis), 3) thermal inertia resulting in lagged responses of water
₁₃₆ temperature to changes in air temperature, 4) incomplete time series data and locations with
₁₃₇ large differences in the amount of available data, 5) spatial and temporal autocorrelation,
₁₃₈ and 6) important predictors of stream water temperature other than air temperature. They
₁₃₉ developed a statistical model that addresses aspects of non-linear relationships, hysteresis,
₁₄₀ thermal inertia, and spatial and temporal autocorrelation but their analysis was limited to a
₁₄₁ single small network of streams with long time series [???].

₁₄₂ We describe a novel statistical model of daily stream temperature that incorporates features
₁₄₃ of stochastic models and extends the Letcher et al. [???] framework to large geographic
₁₄₄ areas. This model handles time series data of widely varying duration from many sites using
₁₄₅ a hierarchical mixed model approach to account for autocorrelation at specific locations
₁₄₆ within watersheds. It incorporates catchment, landscape, and meteorological covariates for
₁₄₇ explanatory and predictive purposes. It includes an autoregressive function to account for
₁₄₈ temporal autocorrelation in the time series, a challenge with other statistical models at fine
₁₄₉ temporal resolution. Additionally, our hierarchical Bayesian approach readily allows for
₁₅₀ complete accounting of uncertainty. We use the model to predict daily stream temperature
₁₅₁ across the northeastern United States over a 36-year time record.

¹⁵² **Methods**

¹⁵³ **Water temperature data**

¹⁵⁴ We gathered stream temperature data from state and federal agencies, individual academic
¹⁵⁵ researchers, and non-governmental organizations (NGOs) from Maine to Virginia (Figure
¹⁵⁶ 1; Table 1?). The data were collected using automated temperature loggers. The temporal
¹⁵⁷ frequency of recording ranged from every 5 minutes to once per hour. This data was
¹⁵⁸ consolidated in a PostgreSQL database linked to a web service at <http://www.db.ecosheds.org>.
¹⁵⁹ Data collectors can upload data at this website and choose whether to make the data publicly
¹⁶⁰ available or not. The raw data is stored in the database and users can flag problem values and
¹⁶¹ time series. Only user-reviewed data are used in the analysis and flagged values are excluded.
¹⁶² For our analysis, we performed some additional automated and visual quality assurance and
¹⁶³ quality control (QAQC) on the sub-daily values, summarized to mean daily temperatures
¹⁶⁴ and performed additional QAQC on the daily values. The QAQC was intended to flag and
¹⁶⁵ remove values associated with logger malfunctions, out-of-water events (including first and
¹⁶⁶ last days when loggers were recording but not yet in streams), and days with incomplete
¹⁶⁷ data which would alter the daily mean. The QAQC webtool used for flagging questionable
¹⁶⁸ data can be found at <http://db.ecosheds.org/qaqc> We also developed an R (ref) package for
¹⁶⁹ analyzing stream temperature data from our database, including the QAQC functions which
¹⁷⁰ can be found at <https://github.com/Conte-Ecology/conteStreamTemperature>. The R scripts
¹⁷¹ using these functions for our analysis are available at https://github.com/Conte-Ecology/conteStreamTemperature_northeast.

¹⁷³ Stream reach (stream section between any two confluences) was our finest spatial resolution
¹⁷⁴ for the analysis. In the rare case where we had multiple logger locations within the same
¹⁷⁵ reach (2,894 locations from 2,413 reaches) recording at the same time, we used the mean
¹⁷⁶ value from the loggers for a given day. In the future, with sufficient within reach data, it

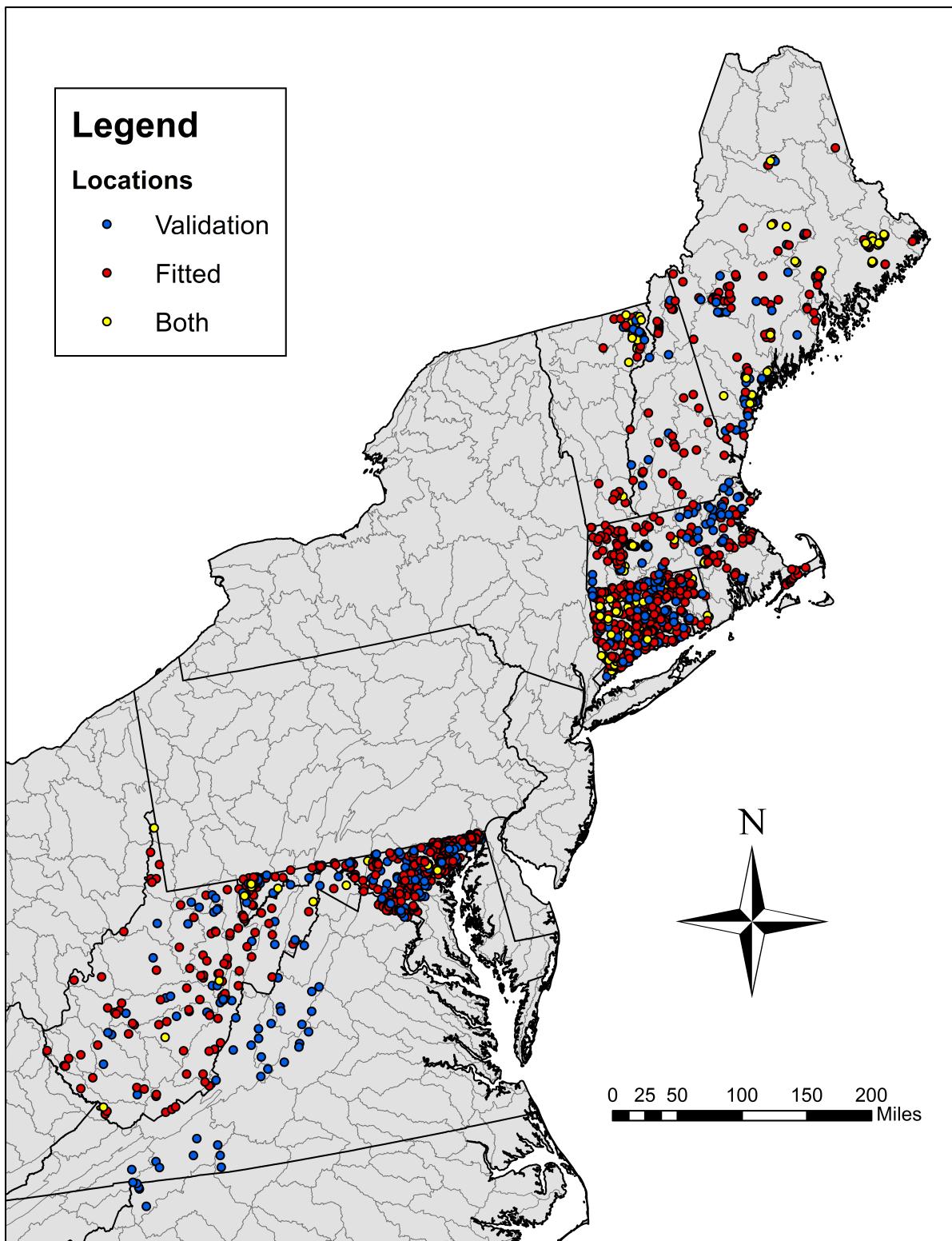


Figure 1: Map of the mean annual maximum 30-day mean stream temperature (mean temperature during the warmest 30-day period each year). The inset shows how much local variation there is that is not clearly visible on the regional map. Gray areas have no predictions, usually because they are in larger streams, outside the bounds of the data used in the model ($>200 \text{ km}^2$ drainage area). Results are presented as catchments delineated based on the stream reaches because at this scale stream lines would blend together and not provide a smooth visual map surface - *not sure if I need to include this, maybe wait to see if*

¹⁷⁷ would be possible to use our modeling framework to also estimate variability within reach
¹⁷⁸ by adding one more level to the hierarchical structure of the model (see Statistical Model
¹⁷⁹ description below).

¹⁸⁰ Table for manuscript??? since we have map and these values don't line up because
¹⁸¹ some sites were missing covariates

state	n_records	n_years	n_locations	n_streams
CT	5,007,479	19	515	418
DE	294,591	10	1	1
MA	3,212,204	20	628	546
MD	258,076	13	497	402
ME	5,522,845	22	274	189
NH	17,191,459	9	151	124
NJ	247,974	4	61	42
NY	6,357,709	20	292	266
PA	17,280,353	10	162	142
RI	2,615	3	4	4
VA	159,334	2	41	41
VT	21,161	13	54	53
WV	835,882	8	214	185
Totals:	56,391,682	22	2894	2413

¹⁸² Stream network delineation

¹⁸³ Temperature logger locations were spatially mapped to the stream reaches of a high resolution
¹⁸⁴ network of hydrologic catchments developed across the Northeastern United States. The Na-
¹⁸⁵ tional Hydrography Dataset High Resolution Delineation Version 2 (NHDHRDV2) maintains

¹⁸⁶ a higher resolution and catchment areal consistency than the established NHDPlus Version 2
¹⁸⁷ dataset. The main purpose of the higher resolution was to capture small headwaters that
¹⁸⁸ may be critical to ecological assessment. A summary of this dataset with links to detailed
¹⁸⁹ documentation can be found in the SHEDS Data project.

¹⁹⁰ **Meteorological and landscape data**

¹⁹¹ The landscape and meteorological data were assembled from various sources. These variables
¹⁹² were spatially attributed to the hydrologic catchments for incorporation into the model
¹⁹³ and include total drainage area, percent riparian forest cover, daily precipitation, daily air
¹⁹⁴ temperature, upstream impounded area, percent agriculture, and percent high-intensity
¹⁹⁵ development. Further descriptions and data sources for each of these variables are described
¹⁹⁶ in Table 1. All of the variables referenced in the table refer to values calculated for the
¹⁹⁷ downstream point of each catchment (confluence pour point).

¹⁹⁸ Table 1. Description and original source of variables used in the model.

Variable	Description	Source
Total Drainage Area	The total contributing drainage area from the entire upstream network	The SHEDS Data project
Riparian Forest Cover	The percentage of the upstream 61 m (200 ft) riparian buffer area that is covered by trees taller than 5 meters	The National LandCover Database (NLCD)
Daily Precipitation	The daily precipitation record for the individual local catchment	Daymet Daily Surface Weather and Climatological Summaries

Variable	Description	Source
Daily Air Temperature	The daily mean air temperature record for the individual local catchment as the mean of the minimum and maximum daily temperature from Daymet	Daymet Daily Surface Weather and Climatological Summaries
Upstream Impounded Area	The total area in the contributing drainage basin that is covered by wetlands, lakes, or ponds that intersect the stream network	U.S. Fish & Wildlife Service (FWS) National Wetlands Inventory
Percent Agriculture	The percentage of the contributing drainage area that is covered by agricultural land (e.g. cultivated crops, orchards, and pasture) including fallow land.	The National LandCover Database
Percent High-Intensity Development	The percentage of the contributing drainage area covered by places where people work or live in high numbers (typically defined as areas covered by more than 80% impervious surface)	The National LandCover Database

¹⁹⁹ **Statistical model**

²⁰⁰ Statistical models of stream temperature often rely on the close relationship between air
²⁰¹ temperature and water temperature. However, this relationship breaks down during the
²⁰² winter in temperature zones, particularly as streams freeze, thereby changing their thermal

203 and properties. Many researchers and managers are interested in the non-winter effects
204 of temperature. The winter period, when phase change and ice cover alter the air-water
205 relationship, differs in both time (annually) and space. We developed an index of air-water
206 synchrony ($Index_{sync}$) so we can model the portion of the year that it not affected by freezing
207 properties. The index is the difference between air and observed water temperatures divided
208 by the water temperature plus 0.000001 to avoid division by zero.

209 We calculate the $Index_{sync}$ for each day of the year at each reach for each year with observed
210 data. We then calculate the 99.9% confidence interval of $Index_{sync}$ for days between the 125
211 and 275 days of the year (05 May and 02 October). Then moving from the middle of the year
212 (day 180) to the beginning of the year, we searched for the first time when 10 consecutive
213 days were not within the 99.9% CI. This was selected as the spring breakpoint. Similarly
214 moving from the middle to the end of the year, the first event with fewer than 16 consecutive
215 days within the 99.9% CI was assigned as the autumn breakpoint. Independent breakpoints
216 were estimated for each reach-year combination. For reach-years with insufficient data to
217 generate continuous trends and confidence intervals, we used the mean break points across
218 years for that reach. If there was not sufficient local reach information, we used the mean
219 breakpoints from the smallest hydrologic unit the reach is nested in (i.e. check for mean
220 from HUC12, then HUC10, HUC8, etc.). More details regarding the identification of the
221 synchronized period can be found in Letcher et al. [??]. The portion of the year between
222 the spring and autumn breakpoints was used for modeling the non-winter, approximately
223 ice-free stream temperatures.

224 We used a generalized linear mixed model to account for correlation in space (stream reach
225 nested within HUC8). This allowed us to incorporate short time series as well as long time
226 series from different reaches and disjunct time series from the same reaches without risk of
227 pseudoreplication (ref: Hurlbert). By limited stream drainage area to $<200\ km^2$ and only
228 modeling the synchronized period of the year, we were able to use a linear model, avoiding

229 the non-linearities that occur at very high temperatures due to evaporative cooling and near
 230 0 C due to phase change [Mohseni and Stefan, 1999]. The general model structure is depicted
 231 in Figure 2.

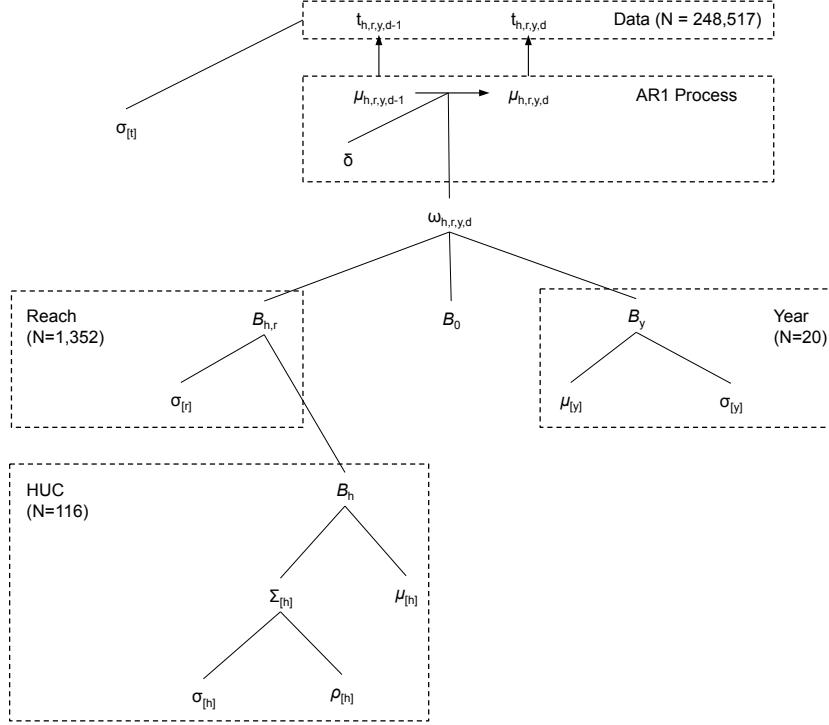


Figure 2: Hierarchical structure of the daily stream temperature model. The observed daily temperatures are $t_{h,r,y,d}$ at HUC8 h and reach r in year y on day d . In general, μ represent means, σ represent standard deviations, B represent vectors of coefficients with subscripts representing the level of variation, Σ is the covariance matrix, ρ is the correlation matrix, ω is the expected temperature as a function of the deterministic components prior to inclusion of temporal autocorrelation, and δ is the autocorrelation coefficient. See details in the text for further description of the coefficients.

232 We assumed stream temperature measurements were normally distributed following,

$$t_{h,r,y,d} \sim \mathcal{N}(\mu_{h,r,y,d}, \sigma_{[t]})$$

233 where $t_{h,r,y,d}$ is the observed stream water temperature at the reach (r) within the sub-basin
 234 identified by the 8-digit Hydrologic Unit Code (HUC8; h) for each day (d) in each year (y).
 235 The expected mean temperature is $\mu_{h,r,y,d}$ and $\sigma_{[t]}$ is the standard deviation. Subscripts
 236 represent the levels at which the value varies. Bracketed subscripts are solely for additional
 237 naming purposes, for example to distinguish means and variances from different levels of the
 238 hierarchical model.

239 The mean temperature is modeled to follow a linear trend

$$\omega_{h,r,y,d} = X_{[0]}B_{[0]} + X_{h,r}B_{h,r} + X_hB_h + X_yB_y$$

240 but the expected mean temperature ($\mu_{h,r,y,d}$) was also adjusted based on the residual error
 241 from the previous day

$$\mu_{h,r,y,d} = \begin{cases} \omega_{h,r,y,d} + \delta(t_{h,r,y,d-1} - \omega_{h,r,y,d-1}) & \text{for } t_{h,r,y,d-1} \text{ is real} \\ \omega_{h,r,y,d} & \text{for } t_{h,r,y,d-1} \text{ is not real} \end{cases}$$

242 where δ is an autoregressive [AR(1)] coefficient and $\omega_{h,r,y,d}$ is the expected temperature before
 243 accounting for temporal autocorrelation in the error structure.

244 $X_{[0]}$ is the $n \times K$ matrix of predictor values. $B_{[0]}$ is the vector of K coefficients, where K
 245 is the number of fixed effects parameters including the overall intercept. We used 15 fixed
 246 effect parameters including interaction terms but not the overall intercept. These were 2-day
 247 total precipitation, 30-day cumulative precipitation, drainage area, upstream impounded
 248 area, percent riparian forest cover, and various two- and three-way interactions (Table 1?).
 249 We assumed the following distributions and vague priors for the fixed effects coefficients

$$B_{[0]} = \begin{pmatrix} \beta_{[1]} \\ \vdots \\ \beta_{[K]} \end{pmatrix} \sim \mathcal{N}(0, 100)$$

250 $B_{h,r}$ is the $R \times L$ matrix of regression coefficients where R is the number of unique reaches
 251 and L is the number of regression coefficients that vary randomly by reach within HUC8. In
 252 this case, we included a random intercept, and random slopes for the air temperature and
 253 7-day air temperature ($L = 3$; Table 1). We assumed prior distributions of

$$B_{h,r} = \begin{pmatrix} \beta_{h,r,[0]} \\ \beta_{h,r,[1]} \\ \beta_{h,r,[2]} \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \sigma_{[r0]}^2 & 0 & 0 \\ 0 & \sigma_{[r1]}^2 & 0 \\ 0 & 0 & \sigma_{[r2]}^2 \end{pmatrix}\right)$$

254 where $B_{h,r}$ is an $R \times L$ matrix, $\beta_{h,r}$ are normally distributed vectors of coefficients with a
 255 mean of 0 and length of R , for the intercept ($\beta_{h,r,[0]}$) and random slopes. We assumed an
 256 independent uniform prior on each standard deviation [Gelman2006],

$$\sigma_{[r]} \sim \text{uniform}(0, 100)$$

257 For the random HUC8 level component, X_h is the matrix of parameters that vary by HUC8.
 258 B_h is the $H \times L$ matrix of coefficients where H is the number of HUC8 groups. We allowed
 259 for correlation among the effects of these HUC8 coefficients as described by Gelman and Hill
 260 [??]. As such, we assumed priors distributions of

$$B_h \sim \mathcal{N}(M_{[h]}, \Sigma_{[h]}), \text{ for } h = 1, \dots, H$$

261 where $M_{[h]}$ is a vector of the means of length L and $\Sigma_{[h]}$ is the $L \times L$ covariance matrix. We

²⁶² assumed the means followed a multivariate normal distribution,

$$M_{[h]} \sim MVN(\mu_{[h(1:L)]}, \sigma_{[h(1:L)]})$$

²⁶³ with a vague normally distributed prior on the means,

$$\begin{pmatrix} \mu_{[h0]} \\ \mu_{[h1]} \\ \mu_{[h2]} \end{pmatrix} \sim \mathcal{N}(0, 100)$$

²⁶⁴ We used a vague inverse-Wishart prior to describe the covariance matrix,

$$\Sigma_{B_h} = \begin{pmatrix} \sigma_{[h0]}^2 & \rho_1 \sigma_{[h0]} \sigma_{[h1]} & \rho_2 \sigma_{[h0]} \sigma_{[h2]} \\ \rho_1 \sigma_{[h0]} \sigma_{[h1]} & \sigma_{[h1]}^2 & \rho_3 \sigma_{[h1]} \sigma_{[h2]} \\ \rho_2 \sigma_{[h0]} \sigma_{[h2]} & \rho_3 \sigma_{[h1]} \sigma_{[h2]} & \sigma_{[h2]}^2 \end{pmatrix} \sim \text{Inv-Wishart}(\text{diag}(L), L + 1)$$

²⁶⁵ where $\sigma_{[h1]}$, $\sigma_{[h1]}$ and $\sigma_{[h2]}$ are the standard deviations of the random HUC8 effects and $\rho_{1:3}$

²⁶⁶ are the correlation coefficients. In addition to random reach and HUC effects, we also allowed

²⁶⁷ for the intercept to vary randomly by year. We assumed a prior distribution of

$$B_y \sim \mathcal{N}(0, \sigma_{[y]})$$

²⁶⁸ for the random year effects with the standard deviation following a vague uniform distribution,

$$\sigma_y \sim \text{uniform}(0, 100)$$

²⁶⁹ To estimate all the parameters and their uncertainties, we used a Bayesian analysis with a

²⁷⁰ Gibbs sampler implemented in JAGS (ref) through R (ref) using the rjags package (ref). This

²⁷¹ approach was beneficial for hierarchical model flexibility and tractability for large datasets.
²⁷² We used vague priors for all parameters so all inferences would be based on the data. We
²⁷³ ran 13,000 iterations on each of three chains with independent random starting values. We
²⁷⁴ discarded the first 10,000 iterations, then thinned; saving every third iteration for a total of
²⁷⁵ 3,000 iterations across 3 chains to use for inference.

²⁷⁶ Model validation

²⁷⁷ To validate our model, we held out 10% stream reaches at random. We also held out 10% of
²⁷⁸ remaining reach-year combinations with observed temperature data at random. Additionally,
²⁷⁹ we excluded all 2010 data because it was an especially warm summer across the northeastern
²⁸⁰ U.S. based on the mean summer daymet air temperatures. This approach was also used by
²⁸¹ [DeWeber and Wagner, 2014a] and helps to assess the model's predictive ability under future
²⁸² warming conditions. This included reaches with no data located within subbasins with and
²⁸³ without data, which will be important if using this model with future climate predictions.
²⁸⁴ The most challenging validation scenario was at reaches within HUC8s without any data in a
²⁸⁵ year without any data. In total, 26.4% of observations and 33.3% of reaches were held out
²⁸⁶ for validation.

²⁸⁷ Derived metrics

²⁸⁸ We use the meteorological data from daymet to predict daily temperatures for all stream
²⁸⁹ reaches (<200 km²) in the region for the synchronized period of the year from 1980-2015.
²⁹⁰ The predictions are conditional on the specific random effects where available and receive
²⁹¹ the mean effect for reaches, HUC8s, and years when no data was collected. From these
²⁹² daily predictions, we derive a variety of metrics to characterize the stream thermal regime.
²⁹³ These include mean (over the 36 years) July temperature, mean summer temperature, mean
²⁹⁴ number of days per year above a thermal threshold (18, 20, 22 C used by default), frequency

295 of years that the mean daily temperature exceeds each of these thresholds, and the maximum
296 7-day and 30-day moving means for each year and across all years. We also calculated the
297 resistance of water temperature to changes in air temperature during peak air temperature
298 (summer) based on the cumulative difference between the daily temperatures. Finally, we
299 assess the thermal sensitivity for each stream reach as the change in daily stream temperature
300 per 1 C change in daily air temperature. This is essentially the reach-specific air temperature
301 coefficient converted back to the original scale from the standardized scale.

302 Results

303 To fit the model, we used 248,517 daily temperature observations from 1,352 stream reaches
304 within 116 HUC8 subbasins over a 21-year period between 1995 and 2015, excluding all
305 records from 2010 for validation.

306 *Evaluation of MCMC convergence (visual and R-hat)*

307 The iterations of the three MCMC chains converged on a single area of high posterior
308 probability while exhibiting minimal autocorrelation, based on visual inspection of the
309 iteration traceplots, partial vs. full density plots, autocorrelation (ACF) plots. The potential
310 scale reduction factors (PSRF, \hat{R}) for all parameters and the multivariate PSRF were < 1.1 ,
311 further indicating good convergence of the MCMC chains [Brooks and Gelman, 1998].

312 *Coefficient estimates from the model*

313 Most variables and their interactions were significant with 95% Credible Intervals (CRI) that
314 did not overlap zero (Table 1). The only non-significant parameters were the interactions
315 of air temperature and forest cover and air temperature and Impounded Area. Drainage
316 area alone was not significant but it was significant in its interactions with all combinations
317 of air temperature and precipitation (Table 1). Air temperature (1-day and 7-day) was the
318 primary predictor of daily water temperature. The effect of air temperature was dampened

³¹⁹ by interactions with precipitation and drainage area (negative 3-way interactions; Table
³²⁰ 1). There was also a large autocorrelation coefficient ($AR1 = 0.77$), indicating that if the
³²¹ other parameters in the model predicted temperature to be over- or under-estimated by 1 C
³²² yesterday, they will be similarly over- or under-estimated by 0.77 C today.

³²³ Table 2. Regression summary table with coefficient estimates including the mean, standard
³²⁴ deviation (SD), and 95% credible intervals (LCRI = 2.5%, UCRI = 97.5%).

³²⁵ **Fixed effects:**

Parameter	Mean	SD	LCRI	UCRI
Intercept	16.69	0.135	16.4182	16.949
AirT	1.91	0.022	1.8620	1.950
7-day AirT	1.36	0.029	1.3015	1.417
2-day Precip	0.06	0.002	0.0546	0.063
30-day Precip	0.01	0.006	0.0005	0.026
Drainage Area	0.04	0.096	-0.1452	0.232
Impounded Area	0.50	0.095	0.3181	0.691
Forest Cover	-0.15	0.047	-0.2455	-0.059
AirT x 2-day Precip	0.02	0.002	0.0195	0.028
AirT x 30-day Precip	-0.01	0.004	-0.0224	-0.007
AirT x Drainage	-0.06	0.029	-0.1170	-0.006
AirT x Impounded Area	0.02	0.029	-0.0345	0.077
AirT x Forest	-0.02	0.015	-0.0508	0.009
2-day Precip x Drainage	-0.04	0.002	-0.0424	-0.034
30-day Precip x Drainage	-0.06	0.006	-0.0709	-0.046
AirT x 2-day Precip x Drainage	-0.01	0.002	-0.0156	-0.008
AirT x 30-day Precip x Drainage	-0.01	0.004	-0.0193	-0.004
AR1	0.77	0.002	0.7681	0.776

³²⁶ Random effects:

Group		Coef	SD	Variance
Site	Intercept	1.03	1.060	
	AirT	0.29	0.083	
	7-day AirT	0.35	0.120	
HUC8	Intercept	0.59	0.345	
	AirT	0.27	0.072	
	7-day AirT	0.26	0.066	
Year	Intercept	0.28	0.076	

³²⁷ HUC8 coefficient correlations:

	Intercept	AirT	7-day AirT
Intercept			
AirT			
7-day AirT	0.338	0.234	

³²⁸ Variability at the reach and huc scales

³²⁹ There was much more unexplained random variation among sites than among HUC8, but the
³³⁰ effects of air temperature on water temperature were only slightly more variable among sites
³³¹ compared with HUC8. There was very little random variability among years not explained
³³² by other parameters (Table 1).

³³³ Evaluation of model fit and predictive power

³³⁴ The overall Root Mean Squared Error (RMSE) was 0.61 C and the residuals were normally
³³⁵ distributed and unbiased (exhibiting no visual heterogeneity), indicating that the model was
³³⁶ a good approximation of the process generating the data. These predicted values are adjusted

337 for residual error, but to understand how well the model predicts temperatures when the
338 previous day's observed temperature is unknown it is better to use the predictions prior
339 to adjusting with the residual AR1 term. The RMSE for the fitted data using unadjusted
340 predictions was 1.08 C. All additional predictions and summaries use the unadjusted values
341 to better understand the predictive abilities of the model.

342 Specifically, to evaluate the spatial and temporal predictive power of our model, we used
343 independent validation data consisting of 100,909 daily temperature observations from 723
344 stream reaches within 101 HUC8 subbasins over 20 years from 1996 to 2015. The overall
345 unadjusted RMSE for all validation data was 2.03 C. Similar to the fitted data, there was
346 no bias in the predictions of the validation data, with the potential exception of slight
347 over-prediction at very low temperatures and possible slight under-prediction at very high
348 temperatures (figure - appendix?).

349 To assess predictive accuracy in warm years without data, we calculated the RMSE for all
350 reaches in 2010 (excluded from model fitting) to be 1.85 C. The RMSE in 2010 for reaches
351 that had data in other years used in the modeling fitting was 1.77 C, whereas reaches that
352 had no data in other years had an overall RMSE of 1.95 C in 2010 (no information about
353 the specific reach or year in a warm year). **these values need to be updated from the**
354 **recent model run**

355 Interestingly, there appears to be only a slight improvement in RMSE with increases in
356 the amount of data used in the model fitting or years of observed data (appendix figure).
357 Similarly, there is no affect of the amount of validation data for a reach on the RMSE estimate
358 of that reach (appendix figure).

359 **Derived metrics**

360 Add summary of derived metrics

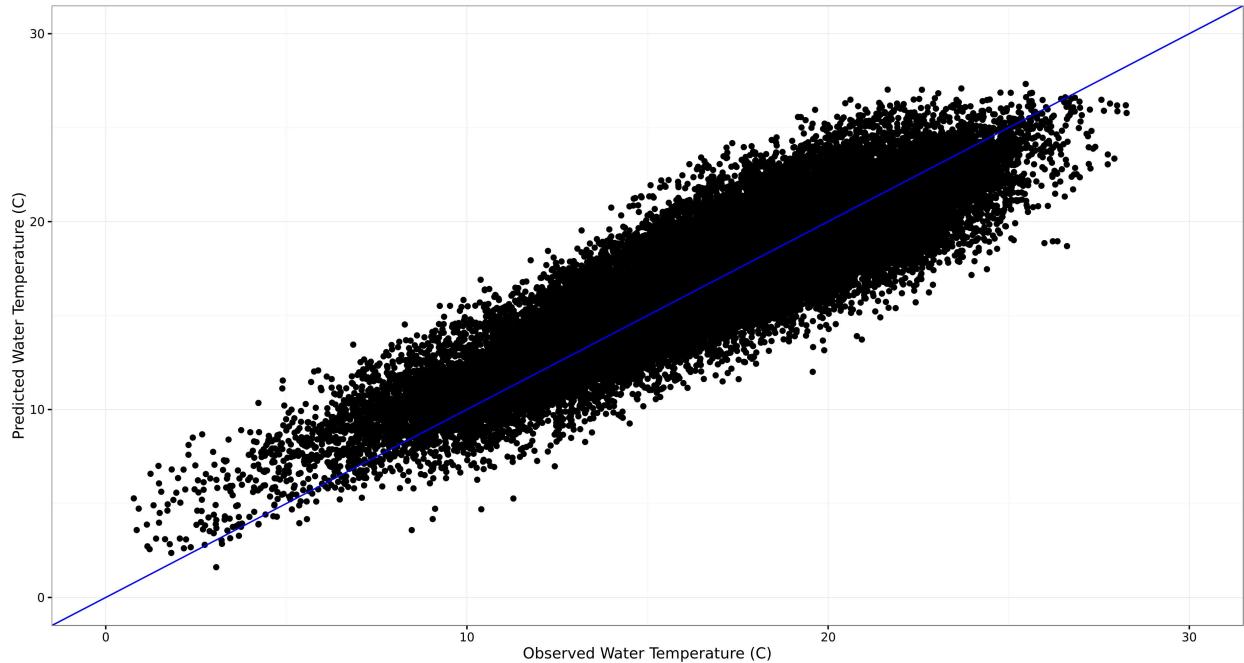


Figure 3: trial text

³⁶¹ Discussion

³⁶² Most aquatic organisms inhabiting streams are ectothermic and are therefore sensitive to
³⁶³ changes in stream temperatures. Although air temperature can be used as a proxy for water
³⁶⁴ temperature in small streams, there is considerable variability in the relationship between
³⁶⁵ air and water temperatures. Additionally, land-use change (e.g. forest cover, impervious
³⁶⁶ surfaces) and modifications to the stream network (e.g. undersized culverts, dams) influence
³⁶⁷ water temperature differently than air temperature. It is also impossible to monitor water
³⁶⁸ temperature across all streams; therefore, regional models are needed to predict stream
³⁶⁹ temperatures across time and space accounting for differences in the landscape and land-
³⁷⁰ use. Many fish biologists have focused on weekly, monthly, or summer-only models of
³⁷¹ stream temperature to relate warm conditions to trout distributions (refs). However, daily
³⁷² temperatures are useful because they can be used in observation processes when activity or
³⁷³ detection is dependent on the current thermal conditions (refs) and they can be summarized
³⁷⁴ into any derived metrics of interest. Depending on the species, life-stage, or management

375 options, decision makers and biologists might be interested in different metrics such as degree
376 days since an event (e.g. oviposition, hatching), frequency of thermal excursions, magnitude
377 of excursions, mean summer temperature, or variability in temperature of different time
378 frames, all of which can be derived from daily temperature predictions. Daily temperatures
379 can also relate more closely to state agency regulations such as the frequency of daily
380 temperatures over a threshold when classifying cold, cool, and warm streams for legal
381 protection (MA Department of Environmental Protection, CALM Regulations, Gerry Szal
382 *personal communication* - should probably find a real reference for this). Without knowing
383 in advance all the potential uses of predicted stream temperatures, a daily model provides
384 the flexibility to derive the values needed for particular decisions.

385 To accommodate these flexible needs, we developed a daily stream temperature model that
386 takes advantage of diverse data sources to make predictions across a large region. Our model
387 fit the data well as indicated by the RMSE < 1 C and had a good ability to predict daily
388 stream temperatures across space and time. With regards to predicting temperatures in
389 warm years without fitted data, such as 2010, the model predicted temperatures well even in
390 reaches with no other data (RMSE = 1.95 C). The predictions were even better at reaches
391 with data from other years (RMSE = 1.77 C), indicating that reach-specific data can improve
392 predictions in future years but this improvement is not dramatic. The lack of dramatic
393 improvement is likely due to multiple factors.

394 Some of the reach-level variability is probably accounted for by other nearby reaches within
395 the same HUC8 (influence of HUC8 random effects). We did not have sufficient data from
396 combinations of reaches, HUC8, and years to compare the RMSE for HUC8 with single versus
397 multiple observed reaches, but based on similar levels of variability explained at the reach
398 and HUC8 levels it is likely that having data from other reaches in a HUC8 improves the
399 predictions for unmonitored reaches in the same HUC8. Therefore, on average, predictions
400 will be worse at reaches within HUC8 with no data. There are also local conditions that

401 vary in time to influence stream temperatures beyond what is included in the model. If the
402 effect of these unmodeled covariates were constant in time, we would expect more of the
403 variation to be captured by the random reach effects and therefore a larger difference in the
404 RMSE in 2010 between reaches with other years of data and reaches with no observed data.
405 Time-varying ground-surface water interactions are likely a major source of the unexplained
406 uncertainty in model predictions. Ground-surface water interactions are particularly complex
407 in the northeastern U.S. and depend on dynamics of precipitation, temperature, snowmelt,
408 local geology, land-use, and landscape physiognomy (refs - I'm just making this up based
409 on physics and basic ecosystem processes). The amount of groundwater entering streams
410 depends on these time-varying conditions but the temperature of the groundwater is also
411 variable, depending on the residence time, depth, and past weather conditions (refs). How
412 much the ground water affects the temperature of the stream water depends of the volume and
413 temperature of each source of water. We do not currently have any landscape or environmental
414 conditions that can predict these ground-surface water interactions over broad space in the
415 northeastern U.S. However, work towards this is in progress and has been applied to other
416 areas (refs: than and others), and any appropriate predictors could be added to our model
417 without needed to change the overall structure of the model.

418 *interpretation of parameter estimates*

419 Of the parameters currently modeled, the current day's air temperature and the mean air
420 temperature over the previous 7 days had the largest effect on daily stream water temperature.
421 This is not surprising as we limited our analysis to small streams and to the synchronized
422 period of the year when air and water temperature are most correlated. Past studies of small
423 streams have also found air temperature to be the main predictor of stream temperature
424 (refs) –compare specific coefficients and TS to other papers?–

425 *partitioning of variability*

426 However, the effects of air temperature and 7-day air temperature were not identical across

space. These effects varied moderately across sites and HUC8 (Table 1), with similar variance for both temperature effects although the daily air temperature had a slightly larger mean effect (Table 1). Additionally, air temperature had significant 3-way interactions with precipitation and drainage area. We used 2-day precipitation x drainage area as an index of flow associated with storms and 30-day precipitation x drainage area as an index of baseflow in these small headwater streams (A. Rosner *personal communication*). Therefore, the negative 3-way interactions with air temperature are what we would expect, indicating that at high flows the effect of air temperature on water temperature is damped. The effect size of these interactions are extremely small, likely in part because of the coarseness of using precipitation x drainage area as an index of flow and not accounting for local ground-surface water interactions.

Air temperature did not interact significantly with percent forest cover or impounded stream area. Alone forest cover had a significant, but small, negative effect on stream temperature during the synchronized period, whereas impounded area had a significant, moderately large positive effect on temperature (Table 1).

We did not include other predictors previously found to be important in statistical models because of correlation with existing covariates or a lack of variability in the potential predictor across the study area. For example, elevation can be a useful predictor of stream temperature (refs) but it lacks a specific mechanistic relationship and covaries strongly with air temperature across the region. Similarly, human development and impervious surfaces can affect stream temperature but in the northeastern U.S. these exhibited high negative correlation with forest cover and both variables could not be included in the model. As more data become available through our data portal <http://db.ecosheds.org>, it may be possible to separate the effects of forest cover and human development variables. Likewise, agricultural land-use can influence stream temperature or the effect of air temperature on stream temperature [??], but there were insufficient observations over a range of agriculture in our data to include

453 it in the current model. Agriculture can be added to a future version of the model as we
454 expand coverage to the mid-Atlantic region of the U.S. and as more data is added to our
455 database. Shading can also influence local stream conditions but is challenging to quantify
456 over large regions. As a step in this direction it would be possible to replace forest cover
457 at the catchment or watershed scale with canopy cover within a riparian buffer area. Both
458 riparian and drainage-level forest cover could be included in the model if there were sufficient
459 data and they were not overly correlated.

460 *Disagreement (conflicting evidence? confused terminology) regarding the drivers of stream*
461 *temperature*

462 *Benefits of our approach*

463 **relate it to the 6 challenges of statistical models the ben describes**

464 *Letcher et al. [2015] outline six general challenges of statistical stream temperature models*
465 *including accounting for 1) the non-linear relationship between air and water temperature at*
466 *high and low air temperatures, 2) different relationships between air and water temperature*
467 *in the spring and fall (hysteresis), 3) thermal inertia resulting in lagged responses of water*
468 *temperature to changes in air temperature, 4) incomplete time series data and locations with*
469 *large differences in the amount of available data, 5) spatial and temporal autocorrelation, and*
470 *6) important predictors of stream water temperature other than air temperature.*

471 Our model addresses a number

472 lots of sensors because relatively cheap and easy to collect, but varying lengths of time at
473 different reaches. Our model incorporates reaches with any length of time (a few days to
474 decades). reaches will little data contribute less to the model but do provide some local
475 and spatial information. The more data a location has the more informative so there is less
476 shrinkage to the mean values. reaches with no data can be predicted based on covariate
477 values and HUC-level random effects but do not get reach-specific coefficient effects.

478 model separates uncertainty in estimates and predictions from variability across space and
479 time. The random reach, HUC, and year effects explicitly address spatial and temporal
480 variability, allowing for more proper accounting of uncertainty.

481 *limitations*

482 ground-surface water interactions not included. However, if remotely sensed predictors could
483 be developed, or exist in a particular region, they could easily be included as site-level
484 predictors.

485 *future developments*

- 486 • groundwater
- 487 • within reach variability
- 488 • autoregressive temperature not just residuals
- 489 • detailed effects of impoundments (exponential decay with distance)
- 490 • spatial autocorrelation
- 491 • expand to larger spatial extent
- 492 • nonlinear relationships
- 493 • model winter
- 494 • adjust breakpoint sync function to adjust with different stream conditions, elevations,
495 and locations
- 496 • dynamic model (effect of air temperature varies over time)

497 *derived metrics*

498 We used the daymet air temperature and precipitation along with landscape covariates to
499 predict daily stream temperatures in each reach then calculated derived metrics of potential
500 interest to biologists, managers, and policy makers.

501 We generated maps of mean derived metrics from temperatures predicted over the daymet
502 record (1980-2013). When scaled to view the entire region the patterns generally follow air

temperature patterns with cooler temperatures at higher elevations and latitudes and warmer temperatures in urban, coastal, and lowland areas. An example of this can be seen on the annual 30-day maximum of the mean daily stream temperature map. However, when zoomed in to view individual catchments on the HUC8 or HUC10 scale, it is clear that there is considerable local variation in water temperatures (Figure #) based on forest cover, drainage area, and local reach effects (unaccounted for local conditions including ground-surface water interactions), as expected based on the model coefficients and past research [Kanno *et al.*, 2013].

In lieu of presenting many small static maps, many of which would look somewhat similar at the regional scale, we added maps of the derived metrics to our web application which can be found at <http://ice.ecosheds.org/>. Users can zoom to specific areas and view information about individual stream reaches and associated catchments. There is also the ability to filter to locate areas with specific conditions. Our main Interactive Catchment Explorer (ICE) for the northeastern and mid-Atlantic regions of the U.S. with information about the landscape conditions and Brook Trout occupancy in addition to stream temperatures can be found at <http://ice.ecosheds.org/> and will be regularly updated as new data become available. This is part of our web platform for Spatial Hydro-Ecological Decision Systems (SHEDS; <http://ecosheds.org/>) where we present visualizations linking datasets, statistical models, and decision support tools to help improve natural resource management decisions. Interested users can contribute, view, and download (if user-designated as publicly available) data at <http://db.ecosheds.org/>. As noted above, these data will be used to further improve model estimates and predictions, which will be presented in ICE.

Although many of the derived metrics relating to peak temperatures have relatively similar broad-scale spatial patterns, there are some metrics that quantify other aspects of the thermal regime. For example, we calculated the resistance of water temperature to changes in air temperature during peak air temperature (summer) based on the cumulative difference

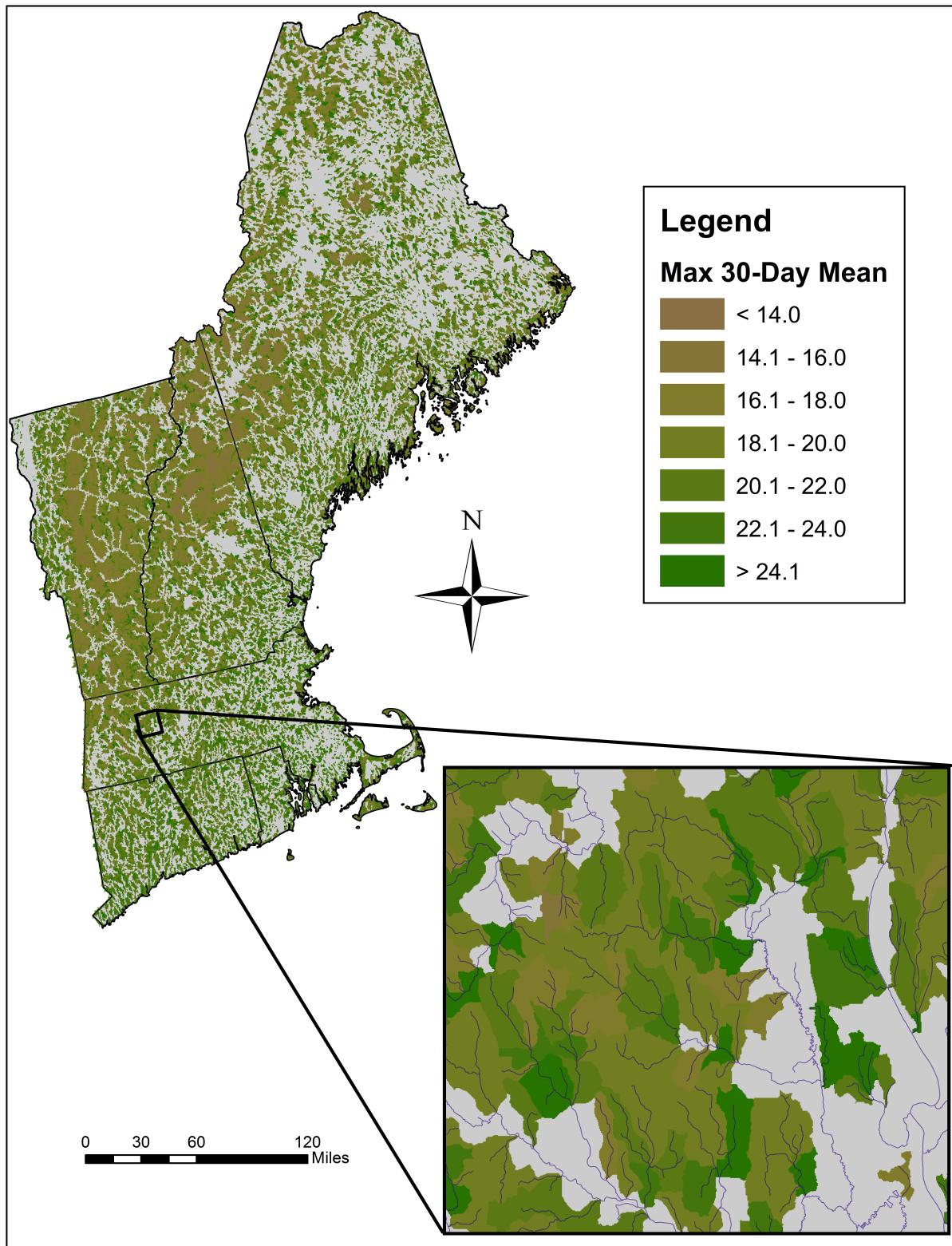


Figure 4: This is an old version and will go down to Virginia when updated

529 between the daily temperatures. The distribution of resistance values was much more right-
530 skewed than the annual 30-day maximum temperature (Figure #). This metric is intended
531 as a potential index of ground water influence on stream temperature. Streams with larger
532 resistance values would be expected to have higher ground water influence because they
533 would essentially be buffered from changes in air temperature during the warmest part of the
534 year (*could make figure to depict this for two extreme cases*). This value could be adjusted
535 for drainage area or flow since it is possible that larger streams always fluctuate less and
536 it could be divided by mean water temperature during the summer to make it reflect the
537 relative resistance. We anticipate future efforts to quantify the influence of ground water
538 in summer stream temperature and explore how well this metric is able to predict those
539 values. Similarly, thermal sensitivity (Figure # - histograms above) or the size of the specific
540 reach random effect could serve as indicators of ground water influence. In particular, the
541 specific reach slope of air temperature suggests that reaches with larger coefficients are highly
542 responsive to changes in air temperature (little ground water buffering) and reaches with
543 small coefficients are insensitive to changes in air temperature and therefore likely to have
544 significant ground water influence. These metrics are hypothesized to indicate ground water
545 influence but remain to be tested. Given the differences in the distributions of these metrics
546 (Figure # histograms), it is likely that some will be considerably more effective as ground
547 water indices than other metrics. A similar effort has recently shown promise in creating a
548 ground water influence index from stream temperature data (ref: snyder, than and colleagues).
549 These indices would currently only apply to reaches with observed data, so the next step
550 would be to find landscape and geological parameters that could predict the best ground
551 water index across the region.

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- 556 Groups who provided data

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