

Water Resources Research



METHOD

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Key Points:

- PASTA is a web application for analyzing paired stream water and air temperature from public and user-owned datasets, even without air data
- The output metrics can evaluate stream thermal sensitivity, relative groundwater contributions, and effective source depth
- Application design allows method consistency and accessibility for various flowing water communities

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Paired Air and Stream Temperature Analysis (PASTA) to Evaluate Groundwater Influence on Streams

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Abstract Groundwater is critical for maintaining stream baseflow and thermal stability; however, the influence of groundwater on streamflow has been difficult to evaluate at broad spatial scales. Techniques such as baseflow separation necessitate streamflow records and do not directly indicate whether groundwater inflow may be sourced from more dynamic shallow flowpaths. We present a web tool application *PASTA* (Paired Air and Stream Temperature Analysis; <https://cuahsi.shinyapps.io/pasta/>) that capitalizes on increased public stream temperature data availability and large-scale, gridded climate observations to provide new and efficient insights regarding relative groundwater influence on streams. *PASTA* analyzes paired air and stream water temperature signals to evaluate spatiotemporal patterns in stream thermal sensitivity and relative groundwater influence, including inference regarding the dominant source groundwater depth (shallow or deep (i.e., approximately >6 m depth)). The tool is linked to publicly available stream temperature datasets and accepts user-uploaded datasets. As local air temperature is not often monitored, *PASTA* pulls daily air temperature data from the comprehensive Daymet products when directly measured data are unavailable, allowing the repurposing of existing stream temperature data. After data are selected or uploaded, the tool (a) fits sinusoidal curves of daily stream and air temperatures by year (water or calendar) to indicate groundwater influence characteristics and (b) performs linear regressions for stream versus air temperatures to indicate stream thermal sensitivity. Results are exported in ASCII file format, creating an efficient and approachable analysis tool for the adoption of newly developed heat tracing analysis from stream reach to landscape scales.

Plain Language Summary Comparing stream temperature to air temperature records can identify streamflow sources, or examine stream vulnerability to land use (e.g., impervious cover), climate change, or river use practices (e.g., dams). We have created a website that allows users to conduct two methods of stream and air temperature comparison using their stream temperature data or use publicly available stream temperature resources in a consistent and accessible format. These analyses generate metrics that indicate similarities and differences in air and stream temperature records over time that can provide insight into hydrologic connectivity for a single site or can be compared across time or space to inform changes in stream process within an area or period of interest.

1. Introduction

Groundwater discharge along the stream corridor is a critical component of many surface water ecosystems, particularly perennial streams and rivers (Boulton & Hancock, 2006; Briggs & Hare, 2018). Aggregate groundwater discharge is a dominant component of baseflow (the portion of the streamflow i.e., sustained between runoff and quickflow events). Baseflow represents a median of 55% of streamflow across the United States and ranges from 14% to 90% (Winter et al., 1998). Stream temperature may show a varied sensitivity to climate change (e.g., Isaak et al., 2016) than expected based on local air temperature change due to numerous factors including groundwater influence (Snyder et al., 2013). Despite their importance, measurements of groundwater discharge are often not readily scalable because they are labor-intensive or depend on extensive streamflow records that are only available at limited sites, with particularly poor coverage in headwater streams (Krabbenhoft et al., 2022). The development of new tools and techniques to rapidly identify streams and rivers with substantial

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groundwater inputs, and spatial variability therein, would increase the capacity of scientists, managers, and other users to identify and prioritize conservation and management (e.g., Gou et al., 2015).

Ecosystem responses to groundwater-surface water interactions are driven not only by the magnitude of groundwater discharge over time but also by the source depths of the discharging groundwater (cumulatively referred to as effective depth; Kurylyk et al., 2015). Groundwater inputs can either impart thermal stability (deeper groundwater) or unexpected variability often due to effects of seasonal shifts on shallower groundwater (e.g., evapotranspiration and dry periods) (Benz et al., 2017; Briggs et al., 2018; Condon, Atchly, et al., 2020; Condon, Markovich et al., 2020; Hare et al., 2021). Shallow groundwater is more directly susceptible to land-use changes (Kurylyk et al., 2015; Taniguchi et al., 2005), climate change (KarisAllen et al., 2022), and surface contamination (Cozzarelli et al., 2020), while older and deeper groundwater may experience natural contamination or contain contaminants from legacy land uses within a watershed (Ransom et al., 2022; Tesoriero et al., 2013). Also, natural chemistry varies laterally and with depth (Condon, Atchly, et al., 2020; Condon, Markovich et al., 2020; Zhi & Li, 2020), which has important implications for surface water quality and stream biogeochemical transformation. Thus, quantifying patterns of discharging groundwater source depth is critical for predicting future stream water supply and quality and facilitating science-based conservation and management decisions.

Comparing co-located air and stream temperatures at seasonal or multi-year timescales can efficiently indicate critical stream temperature processes (Johnson et al., 2020; Kanno et al., 2014; Luce et al., 2014). For example, a linear regression of stream temperature and air temperature may be used to indicate general air-water temperature sensitivity, where air temperature is used as a surrogate for all the cumulative atmospheric controls on stream temperature (Kelleher et al., 2012). However, this approach does not account for time lags between air and stream temperatures. Additionally, paired air-water annual stream temperature signal analysis, which compares the annual sinusoids of air and stream temperatures, requires longer data records but can account for timing differences associated with different groundwater source depths within its output metrics. Thus, it can indicate relative groundwater influence and whether the source groundwater is from the near-surface zone (<~6 m) or deeper flowpaths (Briggs et al., 2018; Johnson et al., 2020, Figure 1).

The methodology we present here is based on the mixed water column signature resulting from heat advected into streams via groundwater discharge over the year. The annual groundwater temperature signal amplitude is influenced by land surface temperature, the aquifer recharge rate, and thermal properties of the soil, but is often primarily controlled by depth from the land surface. Temperature signal amplitudes decay exponentially with depth (Anderson, 2005; Bundschuh, 1993; Constantz, 2008) and are lagged in phase (or timing) compared to temperatures at the surface based on the downward thermal front velocity. The lag increases with depth until the signal is functionally attenuated (non-measurable annual signal amplitude) in deeper groundwater (Briggs et al., 2018). Once the periodic signal is attenuated no phase or lag can be identified. This gradation in phase lags with depth results in a series of characteristic stream temperature signal trends allowing for the identification of groundwater source depth when compared to trends in local air temperature (Figure 1). However, counter-intuitively, shallow groundwater contribution produces a greater phase lag in stream temperature annual signals than deep groundwater due to a greater annual amplitude in the former. Due to the attenuation of groundwater temperature signal with depth and a convergence on mean annual surface temperature, the ratio of means of the air and -water temperature signals show minimal variability due to groundwater inputs, but can indicate heat influences such as geothermal, and anthropogenic modifications (Johnson et al., 2020).

Advances in affordable and reliable temperature loggers are facilitating a rapid expansion in stream temperature time series data collected for stream habitat and water quality purposes. Despite the extensive and growing public availability of water temperature data, communities and practitioners often lack the tools and resources to conduct paired air-water temperature analysis, especially when local air temperature data are not readily available. Here, we describe and discuss *Paired Air and Stream Temperature Analysis* (PASTA; <https://cuahsi.shinyapps.io/pasta/>), a new, browser-operated public-domain web application tool that pairs publicly available or user-inputted surface water and air temperature data to output annual temperature signal parameters (e.g., phase lags, amplitude ratios, and ratio of means) and visualize temperature patterns. We expect this tool to be useful to a wide range of users, including groups focused on local and regional river conservation, research, and/or for educational purposes. PASTA is an interactive platform for users to quickly interpret the potential for groundwater influence on stream and river reaches of interest, assess the general thermal sensitivity of stream water, and make inferences regarding source groundwater characteristics and the potential resiliency to change of various cold-water habitats.

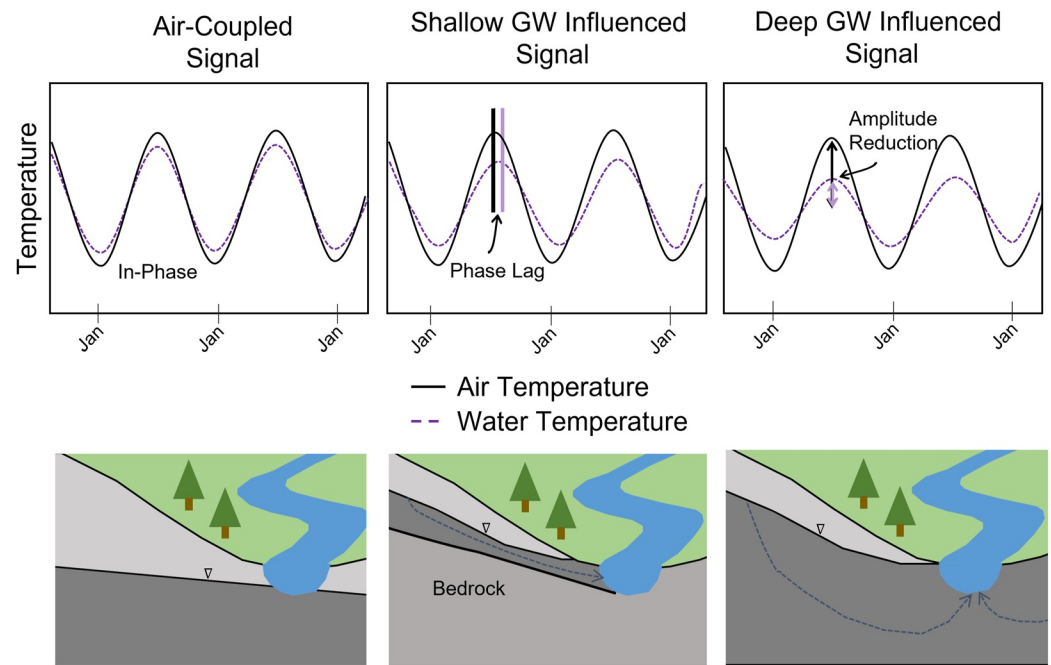


Figure 1. Examples of an annual stream temperature signal compared to the air temperature signal for the three defined paired air-water annual signal classifications over three years (top row) and associated conceptual landscape cross-sections indicating contributing groundwater flowpaths. A stream with substantial deep groundwater (GW) contribution has a strong amplitude reduction, and a stream with a strong shallow GW signal has amplitude reduction and a forward phase shift (i.e., lagged).

2. Methodology

2.1. Software Implementation

Using open-source software R Shiny (Chang et al., 2022), we developed an interactive web application for users to input or access paired surface water and air temperature data to derive annual thermal signal metrics from a sinusoidal curve fitting algorithm (e.g., Briggs et al., 2018; Hare et al., 2021; Johnson et al., 2020, 2021). Our *Paired Air and Stream Temperature Analysis* (PASTA; <https://cuahsi.shinyapps.io/pasta/>) web application is not to be confused with “PASTAS” tool, which uses the open-source scripting language Python for time series modeling of groundwater levels (Collenteur et al., 2019). PASTA calculates the linear regression of daily water temperature versus air temperature, the slope of which can be interpreted as a general metric of stream water thermal sensitivity and groundwater dominance (Kelleher et al., 2012; Letcher et al., 2016). PASTA provides users with detailed output including annual temperature signal metrics (amplitude ratio, phase lag, and mean temperature ratio), linear regression parameters (slope, intercept and R-squared of fit), and metrics for the annual temperature signal sinusoidal fits. All outputs are available for download. Baseflow regression (based on Gustard et al., 1992) can be performed for locations where stream discharge records are available from the National Water Information System (NWIS; U.S. Geological Survey, 2023) to augment the temperature-based analysis.

2.1.1. Functionality List

PASTA allows users to access stream temperature data from multiple publicly available datasets and upload their own data set (in ASCII format), or access data directly from their personal CUAHSI (Consortium of Universities for the Advancement of Hydrologic Science, Inc.) HydroShare account (hydroshare.org). If not supplied by the user, North American daily air temperature data can be retrieved from the 1 km × 1 km Daymet grid cell nearest to the stream temperature measurement point (Thornton et al., 2020), using the R package “daymetr” (Hufkens et al., 2018) requiring the user to upload site coordinates (WGS 1984 projection). Example input tables are available for download from the PASTA *Information* tab (example data from Boose, 2022b, 2022a), but the software allows for a wide range of input types and adapts to all column naming conventions. Air temperature data must be supplied by the user if the location is outside of the extent of Daymet (i.e., North America). Once

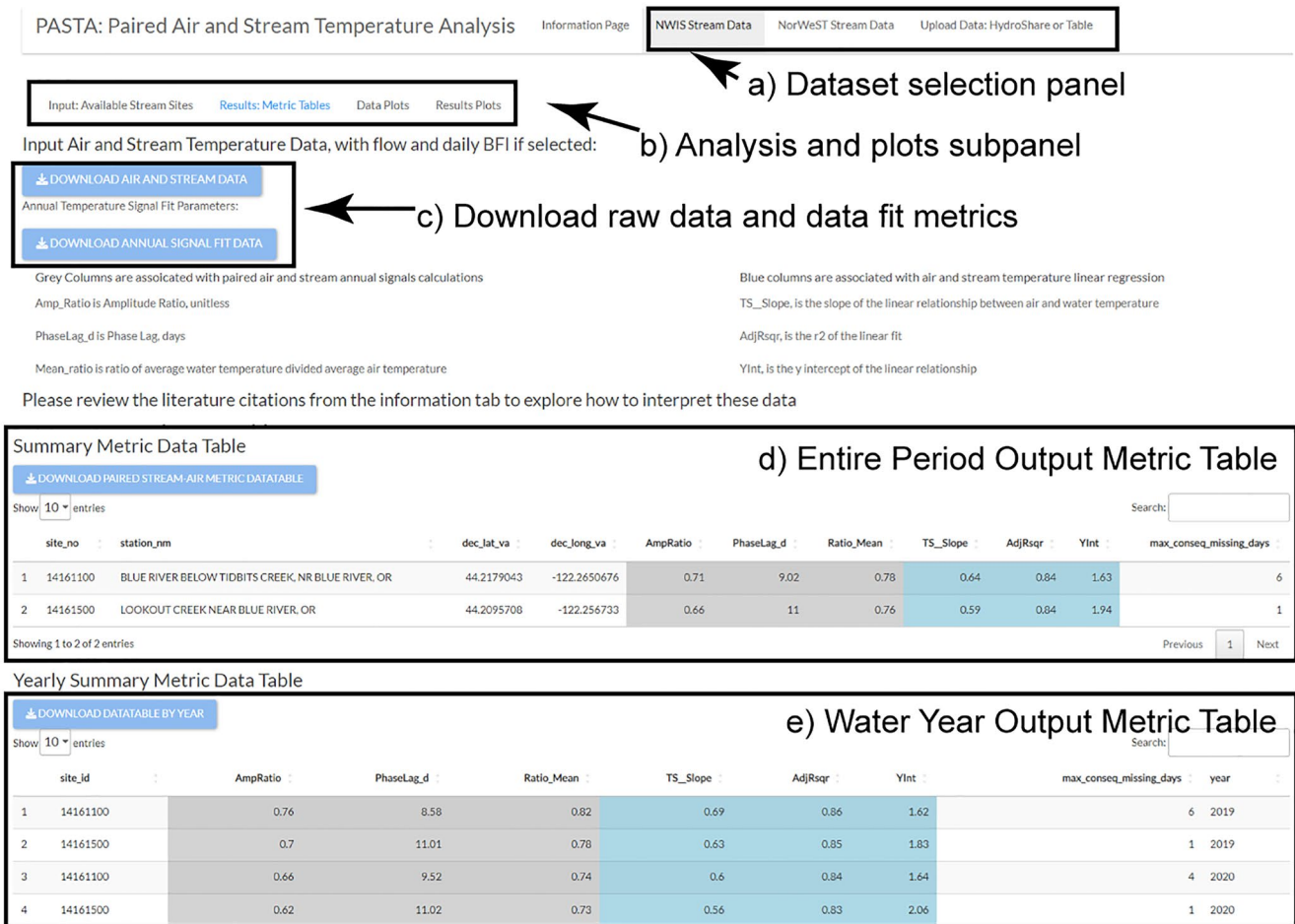


Figure 2. An annotated example of the Paired Air and Stream Temperature Analysis (PASTA) application *Results* tab (second tab within (b)). Within each data set selection (tabset (a)), there is a subtab panel (b) which includes data inputs; result data table, where results are provided as both a summary of user-supplied time period, as well as by each year available; a tab for data plots; and a tab for summary results plots. Results show outputs from Oregon, USA, U.S. Geological Survey (USGS) sites near H.J. Andrews Experimental Forest Watershed where shallow groundwater flowpaths are controlled by shallow bedrock (Herzog et al., 2019). BFI = baseflow indices.

stream temperature and air temperature data are uploaded or selected, these data are organized, erroneous data points are removed, and then data are assessed for completeness. Erroneous data points are defined as water temperature greater than 60°C and air temperature greater than 120°C. Water temperatures less than 1°C are also removed from the analysis because freezing dynamics are inherently non-linear due to the latent heat exchange. We note that high water temperature (>25°C) also imparts a non-linear relationship with air temperature, due to the effects of evaporative cooling (Letcher et al., 2016); however, these data are retained due to the potential use with geothermal-influenced streams and other purposes.

Within the web application, after the user specifies the required inputs for the *Input* tab of the analysis subpanel (Figure 2), the data are processed and available as (a) summary metric tables for the data available within the time period requested, both for the entire time period and by individual water year (*Results: Metric Tables*); (b) time series figures (raw and fit data) for each of the sites with air temperature and stream temperature (*Data Plots*); and, (c) summary metric figures for both the annual thermal signal analysis and linear regression temperature analysis (*Results Plots*). Note “water year” is defined by the USGS as the 12-month period from October 1 to September 30.

While the input data must be quality controlled by the user, a data-completeness parameter is included within the output metric table, with warning colors attributed to data gap time periods exceeding the recommendations of Johnson et al. (2021). Additionally, text and warning colors indicate when phase lags are greater than 40 days

(Figure 2), which can indicate anthropogenic stream management, notably upstream dam presence, and should not be used to infer groundwater connectivity (Hare et al., 2021). However, these data can still be useful depending on the study objectives and are reported as outputs.

Finally, the user may optionally choose to calculate daily baseflow indices (BFI), which are computed using NWIS streamflow data. Data for the selected sites are downloaded from NWIS, and discharge data are assessed for completeness and filled for time periods less than 14 days using the interpolation specifications (based on Elshorbagy et al., 2000) of the “fillMissing” function within the smwrBase R package (Lorenz, 2015). If these discharge data are continuous for the time period requested following this step, a baseflow regression analysis is performed using the “bfi” function from the DVStats R package (Lorenz, 2017). Discharge data are then made available for the user under the download raw data option, which is indicated in item (c) of Figure 2.

2.2. Linear Regression Model Methodology

The paired air and stream linear regression model is conducted using mean daily air and stream data, with an option to perform the regression on weekly data. The regression analysis yields regression slope (TS_slope, °C/°C) and intercept (YInt, °C); these nomenclatures align with the model outputs. The slope is often referred to as the thermal sensitivity, indicating that as the slope deviates away from 1 toward 0, heat fluxes at the atmosphere-stream interface exert less control on stream temperature. However, this method does not account for differences in timing due to the intrinsic thermal properties of these media and shallow groundwater influence. Therefore, this approach can underestimate the strength of the air-water relationship, but often longer time-scale (i.e., weekly and monthly) averages can be used to decrease this limitation (Alexander & Caissie, 2003; Caissie, 2006). The coefficient of determination (r^2) is also reported as a metric output, as this metric can be used to indicate how well air temperature (T_a) can be used to approximate stream water temperature (T_w , Kelleher et al., 2012).

$$T_w = \text{YInt} + \text{TS_slope} \times T_a \quad (1)$$

The linear air-stream temperature relationship can be compared at seasonal timescales using output data, indicating important sub-annual shifts in environmental factors, such as shading or changes to groundwater flux magnitude. An advantage is that this method allows for smaller datasets that do not capture a full year as is required for annual thermal signal analysis. Additionally, this air-water temperature sensitivity metric can quickly indicate where more simple stream temperature modeling approaches might apply (air and water temperature tightly coupled) or where more complex heat budget models should be considered.

2.2.1. Annual Temperature Signal Fit

For a single location, a linearized static sinusoid (Equation 2) is fit to the stream temperature over the period of interest by minimizing the root mean square error (RMSE) of the average daily temperature residuals (°C), and then a separate sinusoid is fit to the local air temperature over the same time period. Note that although PASTA allows annual signal fitting for any time period of interest, the computed metrics are potentially unreliable for less than 1 complete year of data. These fit parameters are available to the user through the “download annual signal fit data” (see (c) of Figure 2).

$$T(t) = a \sin(\omega t) + b \cos(\omega t) + c \quad (2)$$

Here, a , b , and c are regression fit coefficients, ω is the angular frequency (rad/d), t is time (d), and T is either stream or air mean daily temperature. Amplitude (A) and phase (ϕ) for the annual air and stream temperature are calculated using the regression coefficients a and b (Equations 3 and 4, respectively).

$$A = \sqrt{a^2 + b^2} \quad (3)$$

$$\phi = \arctan(b/a) \quad (4)$$

The paired air and stream water signal metrics (amplitude ratio, phase lag, and mean annual temperature ratio) are determined through a comparison of the signal characteristics. Amplitude ratio (A_r) is the ratio of annual stream water temperature signal amplitude to the annual air temperature signal amplitude.

$$A_r = A_w/A_a \quad (5)$$

Table 1

Sample Interpretations of Stream Temperature Metrics Output From Paired Air and Stream Temperature Analysis (PASTA), and Resources to Guide Independent Interpretations

Paired air-stream linear regression output metrics recommended literature: Caissie (2006), Snyder et al. (2013), Kelleher et al. (2012), Letcher et al. (2016)		
Metric	Relative value	Example Interpretation
Linear regression slope	Low (<<1)	Pronounced groundwater influence (e.g., <0.45, Kelleher et al. (2012))
Linear regression intercept	High (>>0, near mean annual air temperature)	Pronounced groundwater influence (e.g., 5°C, Caissie, 2006)
Linear regression r^2	Low (<<1)	Complex temperature dynamics (e.g., <0.6, Kelleher et al. (2012))
Paired Air-Stream Annual Temperature Signal Metric Outputs Recommended Literature: Briggs et al. (2018), Johnson et al. (2020), Hare et al. (2021)		
Metric	Relative value	Example Interpretation
Amplitude ratio	Low (<<1)	Pronounced groundwater influence (e.g., <0.65, Hare et al. (2021))
Phase lag	Negative- (<-10 days)	Problem with data, or flow management
	Negative- (-4 to -10 days)	Review, as could be caused by non-local air temperature data
	Low (-4 to 10)	Deep groundwater or air-coupled, depending on the amplitude ratio (Hare et al., 2021)
	Medium+ (10–40 days)	Shallow groundwater influence (Hare et al., 2021)
Mean Ratio	High+ (>40 days)	Stream management/dams (Hare et al., 2021)
	High (>>1)	Geothermal influence, anthropogenically influenced streams, or non-representative air temperature (e.g. >3.5 for geothermal sites, Johnson et al. (2020))

Note. Relative values are supplied as examples only, as other anthropogenic processes (e.g., dams) can also lead to low linear slope or low amplitude ratios.

Phase lag (ϕ_L) is calculated as the water temperature signal phase subtracted by the air temperature signal phase (Equation 6). Therefore, a positive phase lag indicates air temperature responding faster to atmospheric heat inputs than surface water, which is expected due to the intrinsic thermal properties of these media. Phase is converted from radians to day-of-year using $3\pi/2 - \arctan(b/a)$ (Johnson et al., 2021).

$$\phi_L = \phi_w - \phi_a \quad (6)$$

Negative phase lags can be due to regulated streams, geothermal heating, anthropogenic inputs, or more often from mismatches with local stream temperature and more regional (and/or interpolated) air temperature. When air temperature is measured bankside in natural stream systems negative phase lags are rarely observed (Johnson et al., 2020). Based on the United States continental scale data of Hare et al. (2021), phase lag values less than -4 days should be manually reviewed and less than -10 days indicate data inconsistencies. The mean temperature ratio, or mean ratio (M_r ; Equation 7), can reflect a range of watershed factors. Mean annual groundwater temperature is often close to mean annual stream temperature (Anderson, 2005; Ward, 1985), so this ratio should be near 1 (~0.9–1.1) for most stream sites. The ratio may be slightly higher than 1 for warmer regions, and slightly lower for colder regions due to seasonal flow dynamics (Johnson et al., 2020). Anomalous deviation from 1 can indicate unique processes, such as geothermal influence, anthropogenic influence, or data inconsistencies, often due to poor alignment with air data (Table 1).

$$M_r = M_w/M_a \quad (7)$$

2.3. Data Interpretation: Determining Thresholds

Categorizing stream locations using quantitative scales or classification thresholds of the paired air-water stream temperature metrics is often useful to infer groundwater influence and general thermal sensitivity. Thresholds should be informed by a process-based understanding of paired groundwater and surface water mixing thermodynamics, as detailed by Briggs et al. (2018). We stress that the classifications in Table 1 provide guidance for interpretation, but often “mixed” groundwater sources systems or near-threshold sites are observed, and such complexity is not well captured with static thresholds. Therefore, a classification of shallow or deep groundwater signature does not imply that only one source depth is contributing streamflow, but rather indicates the effective depth that the stream thermal signature reflects (Kurylyk et al., 2015). Likewise, “air-coupled” annual

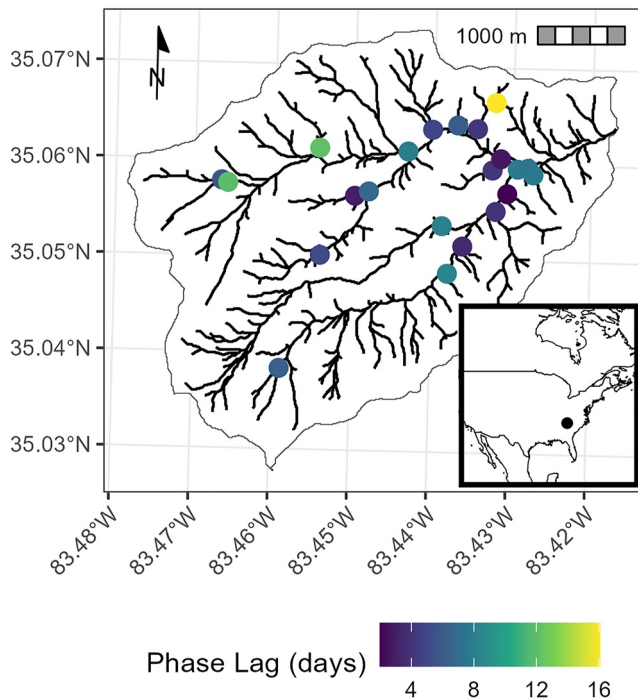


Figure 3. Spatial plot of Coweeta Creek Watershed, North Carolina, USA (16.3 km² drainage area). Circles indicate temperature logger locations and color denotes phase lag (days). Longer phase lags (yellow and green) tend to occur in headwater tributaries.

temperature signals do not indicate a complete lack of groundwater contributions, but rather that the stream thermal regime is dominated by atmospheric heat inputs. When considering the three paired air-stream annual temperature categories “air-coupled,” “shallow groundwater,” and “deep groundwater” signatures, the user should consider the heat budget processes dominating each (as described in detail by Caissie (2006), Johnson et al. (2020), and Kelleher et al. (2012)) and also include connectivity to large natural surface water features such as wetlands and lakes.

Thresholds used by Hare et al. (2021) were based on observations from known deep and shallow sourced stream sites and numerical heat budget modeling of shallow groundwater temperature and conservative groundwater/surface water end-member mixing models developed by Briggs et al. (2018). Also, Johnson et al. (2020) assessed the stream thermal regime categories observed in Maheu et al. (2016) using the paired air-water annual temperature patterns and discussed the nuances between these categories. A basic interpretation of what each variable could indicate, and resources that can provide further interpretation guidance is presented herein (Table 1) to provide high-level overview on interpreting these output metrics.

3. Example Applications of PASTA

PASTA was designed to improve and broaden access to paired air and stream temperature methods, especially as stream temperature data collection efforts increase. This method can be used for single sites but is particularly informative when used to infer patterns among multiple sites. Here we provide two examples of using PASTA for multiple sampling locations (a) within a watershed and (b) longitudinally along a known groundwater-dominated stream.

3.1. Evaluate Watershed Hydrologic Heterogeneity

Heterogeneities in thermal metrics are often observed within a single watershed (Hare et al., 2021), which can indicate variation in groundwater connectivity and groundwater source characteristics among tributaries and along mainstem stream channels. In this example, we used paired air and stream temperature datasets collected in the Coweeta Creek watershed in Otto, NC (Figure 3; Cummins et al., 2022; Miniati et al., 2015) as an example to identify areas with substantial deep versus shallow groundwater dependency. The Coweeta Creek watershed is a Southern Appalachian forested watershed within western North Carolina, USA. This watershed has been the location of nearly a century of stream ecological and hydrological research, after being established in 1934 as a U.S. Department of Agriculture Research Station (Elliott & Vose, 2011). We applied PASTA to the stream and air temperature datasets collected between 2017 and 2019 in 22 stream locations within the Coweeta Creek watershed (Cummins et al., 2022) and observed strong phase lag variability, ranging from 3 to 16 days (Figure 3). Relatively shorter phase lags (4–8 days) tended to occur along the main stem whereas longer phase lags (8–16 days) tended to occur in headwaters; the longer phase lags indicate areas of increased shallow groundwater dependency (Briggs et al., 2018; Johnson et al., 2020) and therefore more susceptibility to stream warming. The longer phase lags are found in headwater streams and indicate more pronounced connection to shallow groundwater sources and varied intrabasin responses of local stream ecosystems to climate change. This example demonstrates the unique hydrologic processes within a single watershed, especially changes to groundwater connectivity and source depth, which may drive punctuated spatial heterogeneity in reliant water quality parameters. These results can then be used to inform sampling plans and targeted research objectives or management practices.

3.2. Groundwater Contribution Variability Along a Stream

Ecologically relevant heterogeneity in groundwater connectivity and air-water temperature sensitivity can also be observed along individual streams. We applied PASTA at high spatial resolution along a 6 km coastal stream reach (six locations; Hurley, 2022) to investigate thermal metric variability in a system that is generally classified

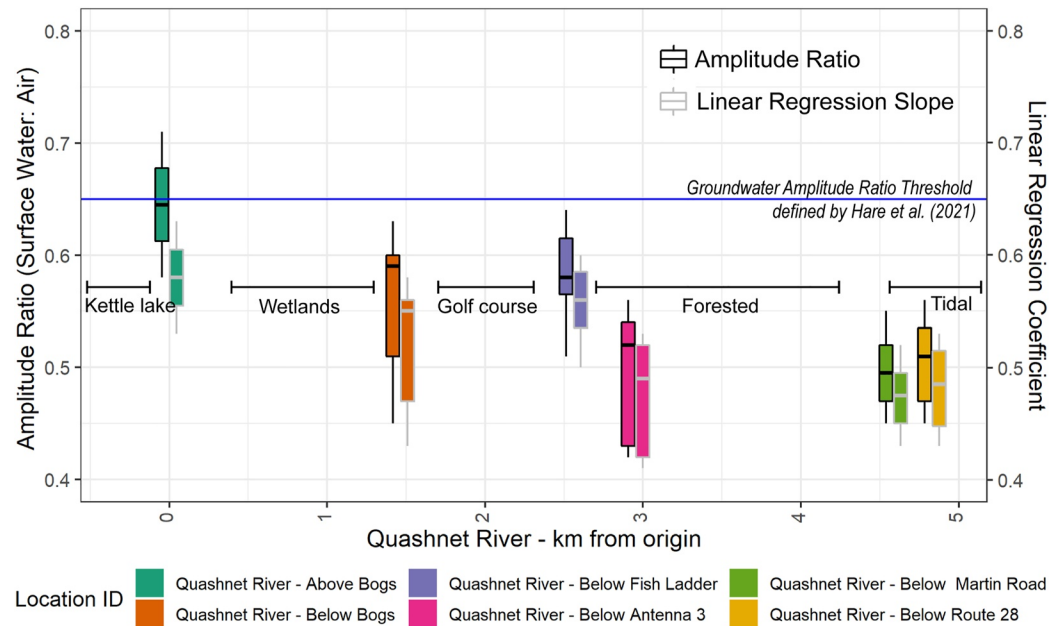


Figure 4. Longitudinal comparison of the amplitude ratio and linear regression coefficient along the Quashnet River, Massachusetts USA, both indicating changes in the thermal influence along the length of the river. Below the blue line (at an amplitude ratio of 0.65) indicates strong groundwater contributions, with lower amplitude ratio values indicating stronger groundwater influence. Amplitude ratio generally decreases along the stream continuum, with the amplitude ratio below the lake representing the strongest seasonal variability and lowest local groundwater influence (predominantly lake water).

as groundwater-dominated, has no major tributaries, and drains a range of land uses. The coastal Quashnet River on Cape Cod, Massachusetts, USA, has been the site of groundwater/surface water exchange research for decades, in part due to its importance as a cold-water brook trout habitat and fishery (Barlow & Hess, 1993), and the presence of groundwater contamination—notably per- and polyfluoroalkyl substances (Briggs et al., 2020). The stream drains an upgradient kettle pond during average to wet periods, but the Quashnet River has no tributaries between the pond and the ocean and an average baseflow index of approximately 0.95 near the downstream extent at U.S. Geological Survey stream gage station 011058837 (Briggs et al., 2020). The influence of historical cranberry farming practices combined with contemporary land uses including a golf course and natural recreation area creates a complex mosaic of groundwater drainage to the stream and potential for spatially variable stream temperature sensitivity.

Observed annual signal phase lags for the Quashnet River stream temperature monitoring sites were less than 9 days and averaged -2 days over 17 years of data. This lack of substantial phase lag is indicative of deep groundwater dominance along the 5 km stream corridor. The relatively high amplitude ratios of the Quashnet River data set found at the monitoring site just below Johns Pond indicate less local groundwater influence and higher stream temperature sensitivity, which may be expected due the direct influence of the larger surface water body, especially during times of higher lake stage (Figure 4). The amplitude ratio metric drops substantially after the stream passes through a groundwater-fed wetland. The river flows through a more densely forested portion of the watershed with an incised stream valley, and amplitude ratios decreases after flowing adjacent to a golf course. That stream reach is known to have strong groundwater discharge influence (e.g., Rosenberry et al., 2016) and is a high-quality brook trout habitat (e.g., Briggs et al., 2018), consistent with our results. Interestingly, the stream corridor amplitude ratio metric patterns are generally mirrored by the linear regression slope metric (Figure 4). However, the linear regression slope alone could not conclusively rule out the influence of shallow groundwater, for which an analysis of phase lag is needed and therefore underestimates air-water relationship. For stream sites with pronounced shallow groundwater or anthropogenic influence we might expect the amplitude ratio and linear slope metrics to diverge (e.g., Briggs et al., 2022), and that is an area of active research using those paired methods.

The Quashnet River example shows that the application of the *PASTA* tool to stream temperature data collected at high spatial resolution (km-scale) can quickly reveal important spatial variability in relative groundwater depth

influence and thermal sensitivity related to local land use and hydrogeology, which can influence stream habitat quality and resiliency, even along streams that are overall dominated by groundwater discharge. Brook trout have been observed seeking cold water in upstream locations near the kettle lake, while brook trout generally do not exhibit that behavior along forested downstream sections (Steve Hurley, Personal Communication 2022). An additional longitudinal km-scale example of using paired air and stream temperature data can be found in Appendix D of Johnson et al. (2020).

4. Conclusions

The publicly available web-tool *PASTA* increases accessibility to quantitative data analysis that offers important insight into the groundwater connectivity of river systems, which has been shown to influence aquatic habitat stability, contamination loading, and overall resilience to extreme events and climate trends. The open-source application enables calculations with two thermal methods using paired air and stream temperatures: annual signals and linear regression, on a platform that greatly improves user accessibility and provides consistent analyses. However, we advocate for the less commonly applied annual signal analysis given the additional information provided regarding groundwater source depth via signal phase lag analysis, while providing similar information regarding thermal sensitivity via signal amplitude ratio analysis (Figure 4). *PASTA* also connects users with publicly available data and allows user-supplied water temperature data to be analyzed with appropriate air temperature data, expanding the usefulness of collected stream temperature data. Our examples emphasize that these data analyses can provide critical insight at varying spatial scales as they can reveal the variability of hydrologic processes within, along, and between streams. Therefore, these tools will allow for more effective river and watershed conservation through facilitating informed sampling plans, restoration efforts, and intentional management strategies. As high-resolution water temperature time series data are relatively ubiquitous given the ease with which water temperature can be measured with inexpensive sensors, the *PASTA* tool makes adding quantitative temperature analysis and interpretation to a watershed community's toolbox to improve hydrologic insight easily accessible.

Data Availability Statement

Version 1.0.3 of *PASTA* is preserved at <https://doi.org/10.5281/zenodo.7808761>, available via MIT license, open-source and developed openly as a R Shiny. All the data used for paired air-stream temperature analysis in this study are available at [HydroShare.org](https://hydroshare.org) via <http://www.hydroshare.org/resource/05799bd0c209449785f401dca6d47728>.

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References

- Alexander, M. D., & Caissie, D. (2003). Variability and comparison of hyporheic water temperatures and seepage fluxes in a small Atlantic salmon stream. *Ground Water*, 41(1), 72–82. <https://doi.org/10.1111/j.1745-6584.2003.tb02570.x>
- Anderson, M. P. (2005). Heat as a ground water tracer. *Ground Water*, 43(6), 951–968. <https://doi.org/10.1111/j.1745-6584.2005.00052.x>
- Barlow, P. M., & Hess, K. M. (1993). *Simulated hydrologic responses of the quashnet river stream-aquifer system to proposed ground-water withdrawals*. Marlborough.
- Benz, S. A., Bayer, P., & Blum, P. (2017). Global patterns of shallow groundwater temperatures. *Environmental Research Letters*, 12(3), 034005. <https://doi.org/10.1088/1748-9326/aa5fb0>
- Boose, E. (2022a). *Fisher Meteorological Station at Harvard Forest since 2001*. *Harvard Forest Data Archive: HF001* (v.27). Environmental Data Initiative. <https://doi.org/10.6073/pasta/a0083f14a6475b78b0bbb2abf26eb295>
- Boose, E. (2022b). *Prospect hill hydrological stations at Harvard forest since 2005*. *Harvard Forest Data Archive: HF070* (v.27). Environmental Data Initiative. <https://doi.org/10.6073/pasta/facbd72c5bee71da4fa8a5fe89574992>
- Boulton, A. J., & Hancock, P. J. (2006). Rivers as groundwater-dependent ecosystems: A review of degrees of dependency, riverine processes and management implications. *Australian Journal of Botany*, 54(2), 133–144. <https://doi.org/10.1071/BT05074>
- Briggs, M. A., Gazoorian, C. L., Doctor, D. H., & Burns, D. A. (2022). A multiscale approach for monitoring groundwater discharge to headwater streams by the U.S. Geological Survey Next Generation Water Observing System Program—An example from the Neversink Reservoir watershed, New York. *Geological Survey Fact Sheet 2022–3077*, 6. <https://doi.org/10.3133/fs20223077>
- Briggs, M. A., & Hare, D. K. (2018). Explicit consideration of preferential groundwater discharges as surface water ecosystem control points. *Hydrological Processes*, 32(15), 2435–2440. <https://doi.org/10.1002/hyp.13178>
- Briggs, M. A., Johnson, Z. C., Snyder, C. D., Hitt, N. P., Kurylyk, B. L., Lantz, L., et al. (2018). Inferring watershed hydraulics and cold-water habitat persistence using multi-year air and stream temperature signals. *Science of the Total Environment*, 636, 1117–1127. <https://doi.org/10.1016/j.scitotenv.2018.04.344>
- Briggs, M. A., Tokranov, A. K., Hull, R. B., LeBlanc, D. R., Haynes, A. B., & Lane, J. W. (2020). Hillslope groundwater discharges provide localized stream ecosystem buffers from regional per- and polyfluoroalkyl substances contamination. *Hydrological Processes*, 34(10), 2281–2291. <https://doi.org/10.1002/hyp.13752>
- Bundschuh, J. (1993). Modeling annual variations of spring and groundwater temperatures associated with shallow aquifer systems. *Journal of Hydrology*, 142(1–4), 427–444. [https://doi.org/10.1016/0022-1694\(93\)90022-2](https://doi.org/10.1016/0022-1694(93)90022-2)

- Caissie, D. (2006). The thermal regime of rivers: A review. *Freshwater Biology*, 51(8), 1389–1406. <https://doi.org/10.1111/j.1365-2427.2006.01597.x>
- Chang, W., J. C., J. A., C. S., B. S., Y. X., et al. (2022). Shiny: Web application framework for R. Retrieved from <https://shiny.rstudio.com/>
- Collenteur, R. A., Bakker, M., Caljé, R., Klop, S. A., & Schaars, F. (2019). Pastas: Open source software for the analysis of groundwater time series. *Groundwater*, 57(6), 877–885. <https://doi.org/10.1111/gwat.12925>
- Condon, L. E., Atchley, A. L., & Maxwell, R. M. (2020). Evapotranspiration depletes groundwater under warming over the contiguous United States. *Nature Communications*, 11(1), 873. <https://doi.org/10.1038/s41467-020-14688-0>
- Condon, L. E., Markovich, K. H., Kelleher, C. A., McDonnell, J. J., Ferguson, G., & McIntosh, J. C. (2020). Where is the bottom of a watershed? *Water Resources Research*, 56(3), e2019WR026010. <https://doi.org/10.1029/2019WR026010>
- Constantz, J. (2008). Heat as a tracer to determine streambed water exchanges. *Water Resources Research*, 44, 1–20. <https://doi.org/10.1029/2008WR006996>
- Cozzarelli, I. M., Kent, D. B., Briggs, M., Engle, M. A., Benthem, A., Skalak, K. J., et al. (2020). Geochemical and geophysical indicators of oil and gas wastewater can trace potential exposure pathways following releases to surface waters. *Science of The Total Environment*, 142909. <https://doi.org/10.1016/j.scitotenv.2020.142909>
- Cummins, C., Hare, D., Bumpers, P. M., Tomczyk, N., Rogers, P., Helton, A., et al. (2022). Coweeta creek watershed stream temperature data. *HydroShare*. <https://doi.org/10.4211/hs.f723219d8cd64aa0aeafc6a8dc46669d>
- Elliott, K. J., & Vose, J. M. (2011). The contribution of the Coweeta Hydrologic Laboratory to developing an understanding of long-term (1934–2008) changes in managed and unmanaged forests. *Forest Ecology and Management*, 261(5), 900–910. <https://doi.org/10.1016/j.foreco.2010.03.010>
- Elshorbagy, A. A., Panu, U. S., & Simonovic, S. P. (2000). Group-based estimation of missing hydrological data, I. Approach and general methodology. *Hydrological Sciences Journal*, 45(6), 849–866. <https://doi.org/10.1080/02626660009492388>
- Gou, S., Gonzales, S., & Miller, G. R. (2015). Mapping potential groundwater-dependent ecosystems for sustainable management. *Groundwater*, 53(1), 99–110. <https://doi.org/10.1111/gwat.12169>
- Gustard, A., Bullock, A., & Dixon, J. M. (1992). *Low flow estimation in the United Kingdom*. Institute of Hydrology.
- Hare, D. K., Helton, A. M., Johnson, Z. C., Lane, J. W., & Briggs, M. A. (2021). Continental-scale analysis of shallow and deep groundwater contributions to streams. *Nature Communications*, 12(1), 1–10. <https://doi.org/10.1038/s41467-021-21651-0>
- Herzog, S. P., Ward, A. S., & Wondzell, S. M. (2019). Multiscale feature - feature interactions control patterns of hyporheic exchange in a simulated headwater mountain stream. *Water Resources Research*, 55, 976–992. <https://doi.org/10.1029/2019WR025763>
- Hufkens, K., Basler, D., Milliman, T., Melaas, E. K., & Richardson, A. D. (2018). An integrated phenology modelling framework in r. *Methods in Ecology and Evolution*, 9(5), 1276–1285. <https://doi.org/10.1111/2041-210X.12970>
- Hurley, S. (2022). *Quashnet river stream temperature data*. HydroShare. Retrieved from <http://www.hydroshare.org/resource/cd003e98225a4408b8012eefad14db2a>
- Isaak, D. J., Young, M. K., Luce, C. H., Hostetler, S. W., Wenger, S. J., Peterson, E. E., et al. (2016). Slow climate velocities of mountain streams portend their role as refugia for cold-water biodiversity. *Proceedings of the National Academy of Sciences of the United States of America*, 113(16), 4374–4379. <https://doi.org/10.1073/pnas.1522429113>
- Johnson, Z. C., Johnson, B. G., Briggs, M. A., Devine, W. D., Snyder, C. D., Hitt, N. P., et al. (2020). Paired air-water annual temperature patterns reveal hydrogeological controls on stream thermal regimes at watershed to continental scales. *Journal of Hydrology*, 587, 124929. <https://doi.org/10.1016/j.jhydrol.2020.124929>
- Johnson, Z. C., Johnson, B. G., Briggs, M. A., Snyder, C. D., Hitt, N. P., & Devine, W. D. (2021). Heed the data gap: Guidelines for using incomplete datasets in annual stream temperature analyses. *Ecological Indicators*, 122, 107229. <https://doi.org/10.1016/j.ecolind.2020.107229>
- Kanno, Y., Vokoun, J. C., & Letcher, B. H. (2014). Paired stream-air temperature measurements reveal fine-scale thermal heterogeneity within headwater brook trout. *River Research and Applications*, 75(6), 745–755. <https://doi.org/10.1002/rra>
- KarisAllen, J. J., Mohammed, A. A., Tamborski, J. J., Jamieson, R. C., Danielescu, S., & Kurylyk, B. L. (2022). Present and future thermal regimes of intertidal groundwater springs in a threatened coastal ecosystem (pp. 4721–4740).
- Kelleher, C., Wagener, T., Gooseff, M., McGlynn, B., McGuire, K., & Marshall, L. (2012). Investigating controls on the thermal sensitivity of Pennsylvania streams. *Hydrological Processes*, 26(5), 771–785. <https://doi.org/10.1002/hyp.8186>
- Krabbenhoft, C. A., Allen, G. H., Lin, P., Godsey, S. E., Allen, D. C., Burrows, R. M., et al. (2022). Assessing placement bias of the global river gauge network. *Nature Sustainability*, 5(7), 586–592. <https://doi.org/10.1038/s41893-022-00873-0>
- Kurylyk, B. L., MacQuarrie, K. T. B., Caissie, D., & McKenzie, J. M. (2015). Shallow groundwater thermal sensitivity to climate change and land cover disturbances: Derivation of analytical expressions and implications for stream temperature modeling. *Hydrology and Earth System Sciences*, 19(5), 2469–2489. <https://doi.org/10.5194/hess-19-2469-2015>
- Letcher, B. H., Hocking, D. J., Neil, K. O., Whiteley, A. R., Nislow, K. H., & Donnell, M. J. O. (2016). A hierarchical model of daily stream temperature using air-water temperature synchronization, autocorrelation, and time lags. *PeerJ*, 1–26. <https://doi.org/10.7717/peerj.1727>
- Lorenz, D. (2017). DVstats: Functions to manipulate daily-values data. R package version 0.3.4.
- Lorenz, D. L. (2015). smwrBase---An R Package for managing hydrologic Data, Version 1.1.1.
- Luce, C., Staab, B., Kramer, M., Wenger, S., Isaak, D., & McConnell, C. (2014). Sensitivity of summer stream temperatures to climate variability in the Pacific Northwest. *Water Resources Research*, 50(4), 3428–3443. <https://doi.org/10.1002/2013WR014329>. Received
- Maheu, A., Poff, N. L., & St-Hilaire, A. (2016). A classification of stream water temperature regimes in the conterminous USA. *River Research and Applications*, 32(5), 896–906. <https://doi.org/10.1002/rra>
- Miniat, C. F., Laseter, S. H., Swank, W. T., & Swift, L. W., Jr. (2015). *Daily air temperature data, recorded by NWS thermometer, from climate station 01 at Coweeta Hydrologic Lab, North Carolina*. Forest Service Research Data Archive. <https://doi.org/10.2737/RDS-2015-0049>
- Ransom, K. M., Nolan, B. T., Stackelberg, P. E., Belitz, K., & Fram, M. S. (2022). Machine learning predictions of nitrate in groundwater used for drinking supply in the conterminous United States. *Science of The Total Environment*, 807, 151065. <https://doi.org/10.1016/j.scitotenv.2021.151065>
- Rosenberry, D. O., Briggs, M. A., Delin, G., & Hare, D. K. (2016). Combined use of thermal methods and seepage meters to efficiently locate, quantify, and monitor focused groundwater discharge to a sand-bed stream. *Water Resources Research*, 52(6), 1–18. <https://doi.org/10.1002/2016WR018808>. Received
- Snyder, C. D., Webb, J. R., Young, J. A., Johnson, Z. B., & Jewell, S. (2013). Significance of headwater streams and perennial springs in ecological monitoring in Shenandoah National Park. Open-File Report 2013–1178, 46.
- Taniguchi, M., Uemura, T., & Sakura, Y. (2005). Effects of urbanization and groundwater flow on subsurface temperature in three megacities in Japan. *Journal of Geophysics and Engineering*, 2(4), 320–325. <https://doi.org/10.1088/1742-2132/2/4/S04>
- Tesoriero, A. J., Duff, J. H., Saad, D. A., Spahr, N. E., & Wolock, D. M. (2013). Vulnerability of streams to legacy nitrate sources. *Environmental Science & Technology*, 47(8), 3623–3629. <https://doi.org/10.1021/es305026x>

- Thornton, M. M., Shrestha, R., Wei, Y., Thornton, P. E., Kao, S., & Wilson, B. E. (2020). Daymet: Daily Surface Weather Data on a 1-km Grid for North America, Version 4. <https://doi.org/10.3334/ORNLDAAC/1840>
- U.S. Geological Survey. (2023). National water information system data available on the World Wide Web (water data for the nation). Retrieved from <http://waterdata.usgs.gov/nwis>
- Ward, J. V. (1985). Thermal characteristics of running waters. *Hydrobiologia*, *125*(1), 31–46. <https://doi.org/10.1007/BF0004592>
- Winter, T. C., Harvey, J. W., Franke, O. L., & Alley, W. M. (1998). *Ground water and surface water; a single resource*. U. S. Geological Survey Circular.
- Zhi, W., & Li, L. (2020). The shallow and deep hypothesis: Subsurface vertical chemical contrasts shape nitrate export patterns from different land uses. *Environmental Science & Technology*, *54*(19), 11915–11928. <https://doi.org/10.1021/acs.est.0c01340>