MacroSheds: a synthesis of long-term biogeochemical, hydroclimatic, and geospatial data from small watershed ecosystem studies

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Authors

Michael Vlah[1] (michael.vlah@duke.edu), Spencer Rhea[1] (spencer.rhea@duke.edu), Emily Bernhardt[1] (emily.bernhardt@duke.edu), Amanda DelVecchia[1] (amanda.delvecchia@unc.edu), Nick Gubbins[2] (nick.gubbins@colostate.edu), Weston Slaughter[1] (weston.slaughter@duke.edu) Audrey Thellman[1] (audrey.thellman@duke.edu), and Matt V. Ross[2] (matt.ross@colostate.edu)

[1]Duke University
[2]Colorado State University

Corresponding author: Matt V. Ross (matt.ross@colostate.edu)

Author Contribution Statement

Bernhardt and Ross originated the project and defined its scope and goals. Vlah, Ross, and Rhea designed the data processing system architecture. Vlah, Rhea, Gubbins, and Slaughter developed the data processing system, with routine feedback from Ross, Bernhardt, and all other authors. Visualizations associated with this paper and the MacroSheds portal were also designed by the full team. Rhea, Vlah, and Slaughter implemented the macrosheds R package. Vlah, Bernhardt, Ross, and Rhea wrote the paper, with edits from the team. Vlah and Rhea generated the figures.

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URL of the Dataset and Metadata with permanent identifier:
https://doi.org/10.6084/m9.figshare.c.5621740
(Dataset will be published at the above URL at the time of manuscript acceptance. Manuscript currently in review at Limnology and Oceanography Letters)

Code URL with permanent identifier: Code repository is at
https://github.com/MacroSHEDS/data_processing

Abstract

The U.S. Federal Government supports hundreds of watershed ecosystem monitoring efforts from which solute fluxes can be calculated. While details of instrumentation and sampling methods vary across these studies, the types of data collected and the questions that motivate their analysis are remarkably similar. Nevertheless, little effort toward the compilation of these datasets has previously been made, and comparative watershed analyses have remained limited in scale. The MacroSheds project has developed a flexible, future-friendly system for continually harmonizing daily time series of streamflow, precipitation, and solute chemistry from 168+ watershed studies across the U.S., and supplementing each with a comprehensive set of predictive watershed attributes. The MacroSheds dataset is an unprecedented resource for watershed ecosystem science, and for hydrology, as a small-watershed supplement to existing collections of streamflow predictors, like CAMELS and GAGES-II. Macrosheds is accompanied by a web dashboard for visualization and an R package for local analysis.

Background and Motivation

Watershed ecosystem science began in the late 1960s, when Herb Bormann and Gene Likens began estimating precipitation inputs and streamwater exports for small gauged watersheds in the Hubbard Brook Experimental Forest (Bormann et al. 1968, 1969). These input and output fluxes and their differences were used to detect trends in air pollution, climate, rates of chemical weathering, nutrient limitation, and nutrient saturation, and to detect the magnitude, duration and severity of disturbance on ecosystem element retention and loss (Likens and Bormann 2013). All of these insights were gained from the consistent comparison of precipitation and streamflow volumes and chemistry conducted over long time scales. The simplicity of the watershed ecosystem approach and the magnitude of its scientific impact has led to similar watershed ecosystem studies being conducted in thousands of watersheds across the globe.

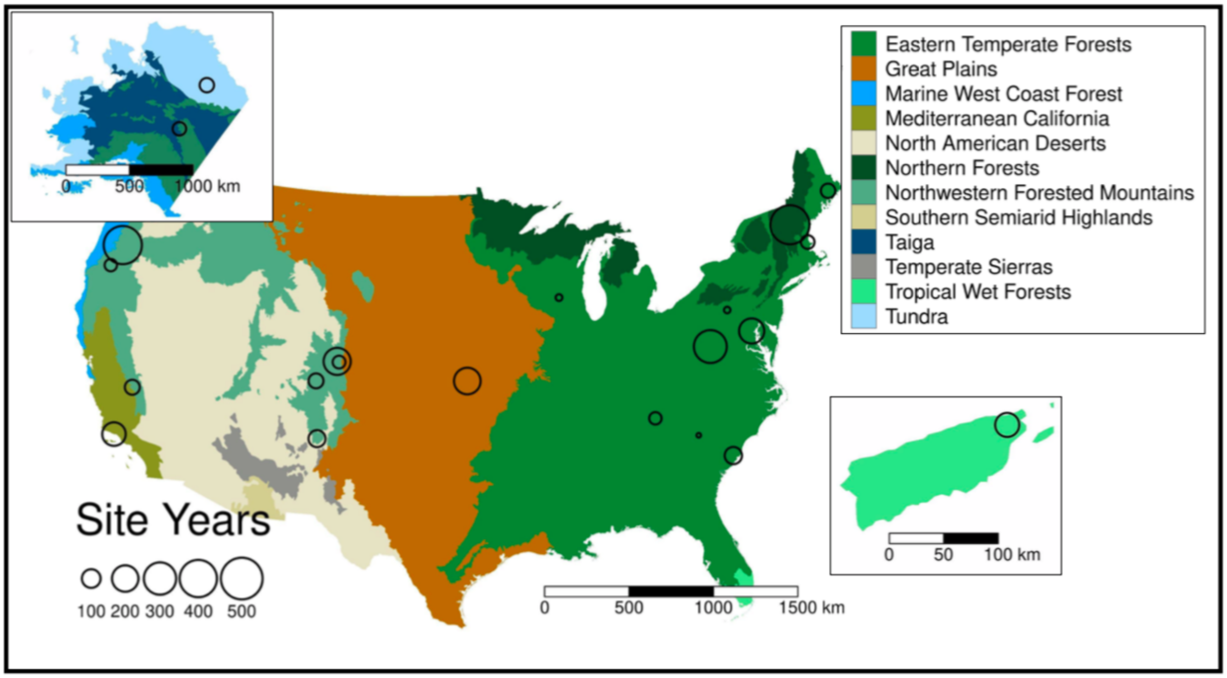


Figure 1. Locations of watershed biogeochemical records included in our initial data synthesis. Colors represent EPA ecoregions.

Collectively, hydrology labs and experimental forests operated by the US Forest Service, Department of Energy, and the National Science Foundation’s Long-term Ecological Research, National Ecological Observatory Network, and Critical Zone Collaborative Network (formerly CZO) programs, support hundreds of small watershed studies around the United States (Figure 1). Each of these programs collects nearly identical types of data. Yet to date, there has been no attempt to collate these datasets into a synthetic data platform that would facilitate comparison across sites. In the notable examples where cross-site analyses have been performed (e.g., Williard et al. 1997; Kaushal et al. 2014; Zhang et al. 2017), they have been limited in spatial scope or applied to only one element (like N) or general water balance. Each of these individual efforts required significant supplemental funding and data expertise to enable synthesis. The challenges inherent to merging even relatively consistent datasets have ultimately limited the scale of inference in watershed ecosystem science.

Indeed, watershed scientists have become increasingly self-critical, recognizing the failure of our community to develop generalities and theories that apply across scales (McDonnell et al. 2007; Kirchner 2009; Lohse et al. 2009). Much of the literature of watershed science over the last decade has focused on gaining ever finer detail on the spatial and temporal heterogeneity of flow paths, water residence times, and biogeochemical processes (McClain et al. 2003; Bernhardt et al. 2017). This fine-scale focus has identified many unique idiosyncrasies of individual watersheds but has not helped us develop general theories about watershed dynamics that can be applied at regional to global scales. It is a fair critique to suggest that most watershed ecosystem studies remain rather parochial, involving detailed studies of individual or paired watersheds, or surveys of a small set of attributes across multiple watersheds. Macroscale watershed science, *or the search for general principles that describe the functional capacity and behavior across watersheds*, has been limited. A major reason for this lack of large-scale focus is the challenge of data access and integration across sites. New requirements for data sharing have made it possible to access most NSF-funded watershed science data, yet individual datasets are rarely interoperable across research sites, even when stored in the same repositories.

We find inspiration for harmonizing large datasets in the hydrology community, where there are two major modern efforts to synthesize records of discharge, precipitation, and watershed/catchment attributes: GAGES-II and CAMELS (Falcone 2011; Newman et al. 2014). Though preeminent examples of data aggregation and distribution, these datasets are limited in their scope to physical hydrology, mostly in watersheds too large to apply the watershed ecosystem concept (Figure 2; Bormann and Likens 1969). Still, these efforts provide a roadmap for synthesizing analysis-ready data for macroscale watershed ecosystem work. With 500 combined citations, they also demonstrate the value of such syntheses to the hydrology community. These datasets have enabled foundational shifts in the ways we make predictions at scale, especially through recent machine-learning advances in rainfall-runoff modeling (Kratzert et al. 2018; 2022). MacroSheds opens this landscape of opportunity to the biogeochemistry community. See the “Comparison with Existing Datasets” section below for more details on how MacroSheds relates to and supplements CAMELS and GAGES-II.

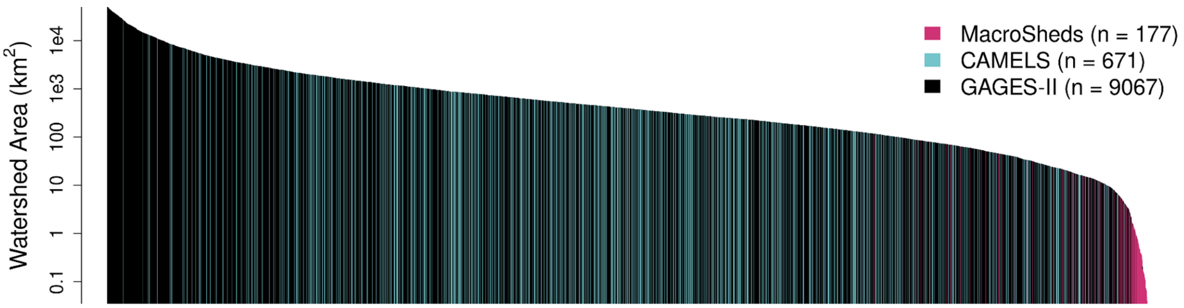
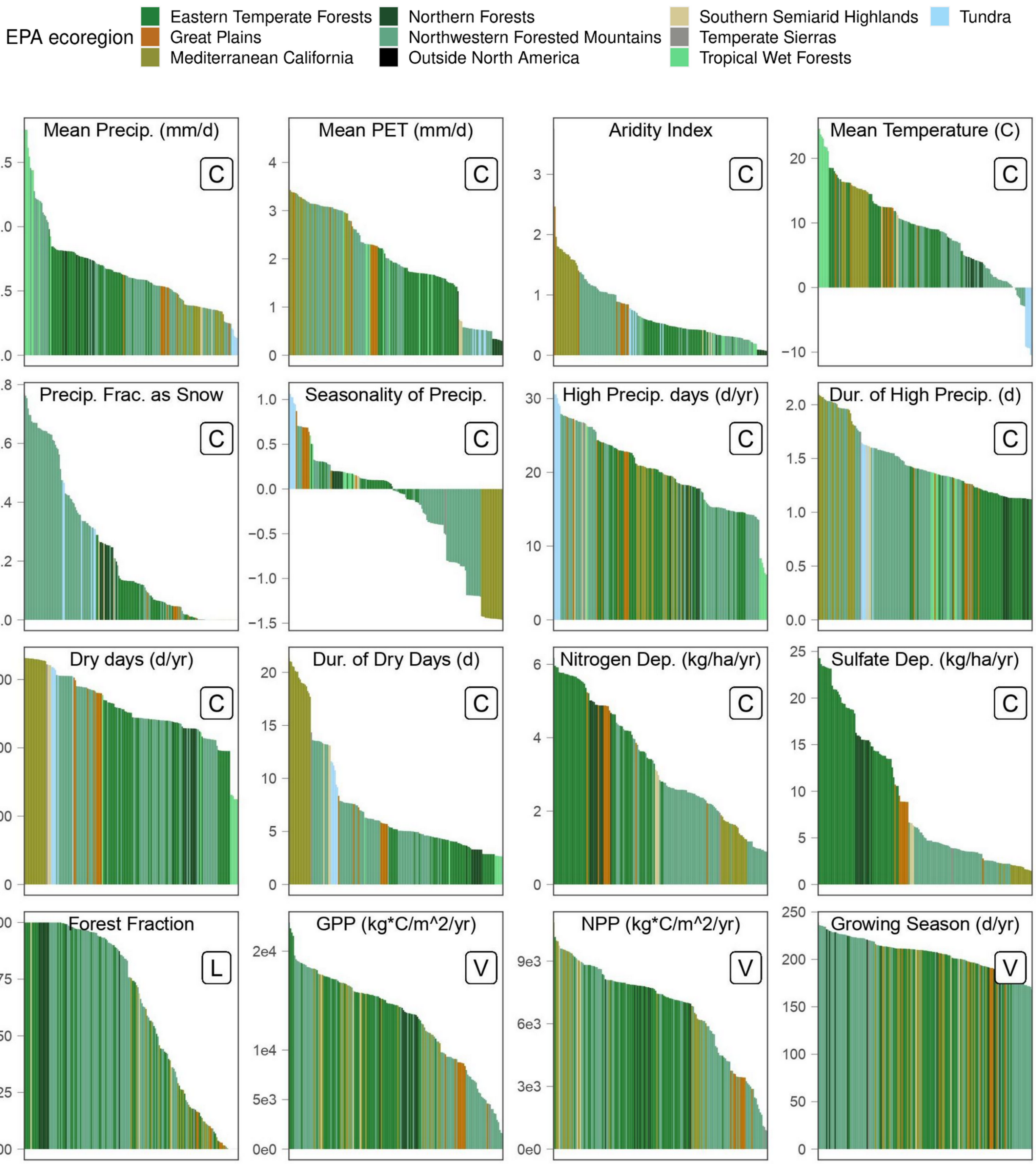


Figure 2. Comparison of watershed areas as represented in the MacroSheds, CAMELS, and GAGES-II datasets. Each vertical bar represents a single watershed. MacroSheds fills out two orders of magnitude at the small end. Note that only those MacroSheds sites for which discharge data are publicly available are included in this figure.

Remote sensing enables macroscale watershed analysis

In this dataset, we unified publicly available data records of precipitation, streamflow, precipitation chemistry, and stream chemistry from watershed ecosystem studies that meet a requirement of at least monthly stream chemistry sampling. We used a common procedure to delineate the watersheds of all stream sampling sites, and PRISM and Daymet to provide standardized estimates of climatology for each site. For each delineated watershed we summarized publicly available, gridded products encompassing topography, geology, soil, vegetation, and landcover attributes. Below we include distributions of hydrology, chemistry, and watershed attributes for 168 stream sampling locations (Figure 3; Figure 4) and correlations between watershed attributes and stream chemical constituents (Figure 5).


EPA ecoregion
Eastern Temperate Forests
Great Plains
Mediterranean California
Northern Forests
Northwestern Forested Mountains
Outside North America
Southern Semiarid Highlands
Temperate Sierras
Tropical Wet Forests
Tundra
Mean Precip. (mm/d)
C
0.0
2.5
5.0
7.5
Mean PET (mm/d)
C
0
1
2
3
4
Aridity Index
C
0
1
2
3
Mean Temperature (C)
C
−10
0
10
20
Precip. Frac. as Snow
C
0.0
0.2
0.4
0.6
0.8
Seasonality of Precip.
C
−1.5
−1.0
−0.5
0.0
0.5
1.0
High Precip. days (d/yr)
C
0
10
20
30
Dur. of High Precip. (d)
C
0.0
0.5
1.0
1.5
2.0
Dry days (d/yr)
C
0
100
200
300
Dur. of Dry Days (d)
C
0
5
10
15
20
Nitrogen Dep. (kg/ha/yr)
C
0
2
4
6
Sulfate Dep. (kg/ha/yr)
C
0
5
10
15
20
25
Forest Fraction
L
0.00
0.25
0.50
0.75
1.00
GPP (kg*C/m^2/yr)
V
0e0
5e3
1e4
2e4
NPP (kg*C/m^2/yr)
V
0e0
3e3
6e3
9e3
Growing Season (d/yr)
V
0
50
100
150
200
250

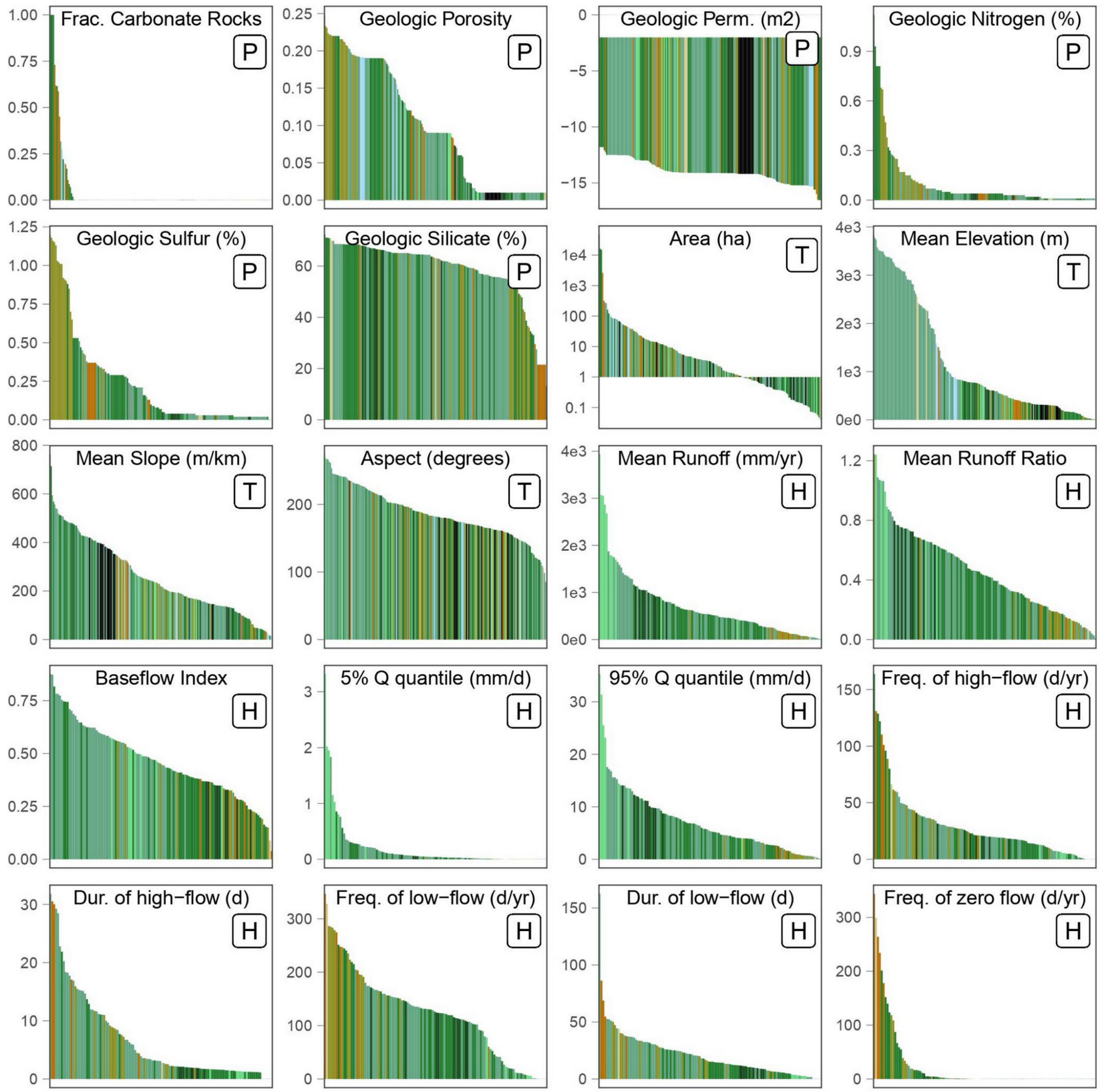


Figure 3. Distributions of watershed attributes across MacroSheds sites. Each vertical bar represents a single site. Inset letter codes stand for attribute categories: Climate, Vegetation, Parent material, Terrain, Hydrology.

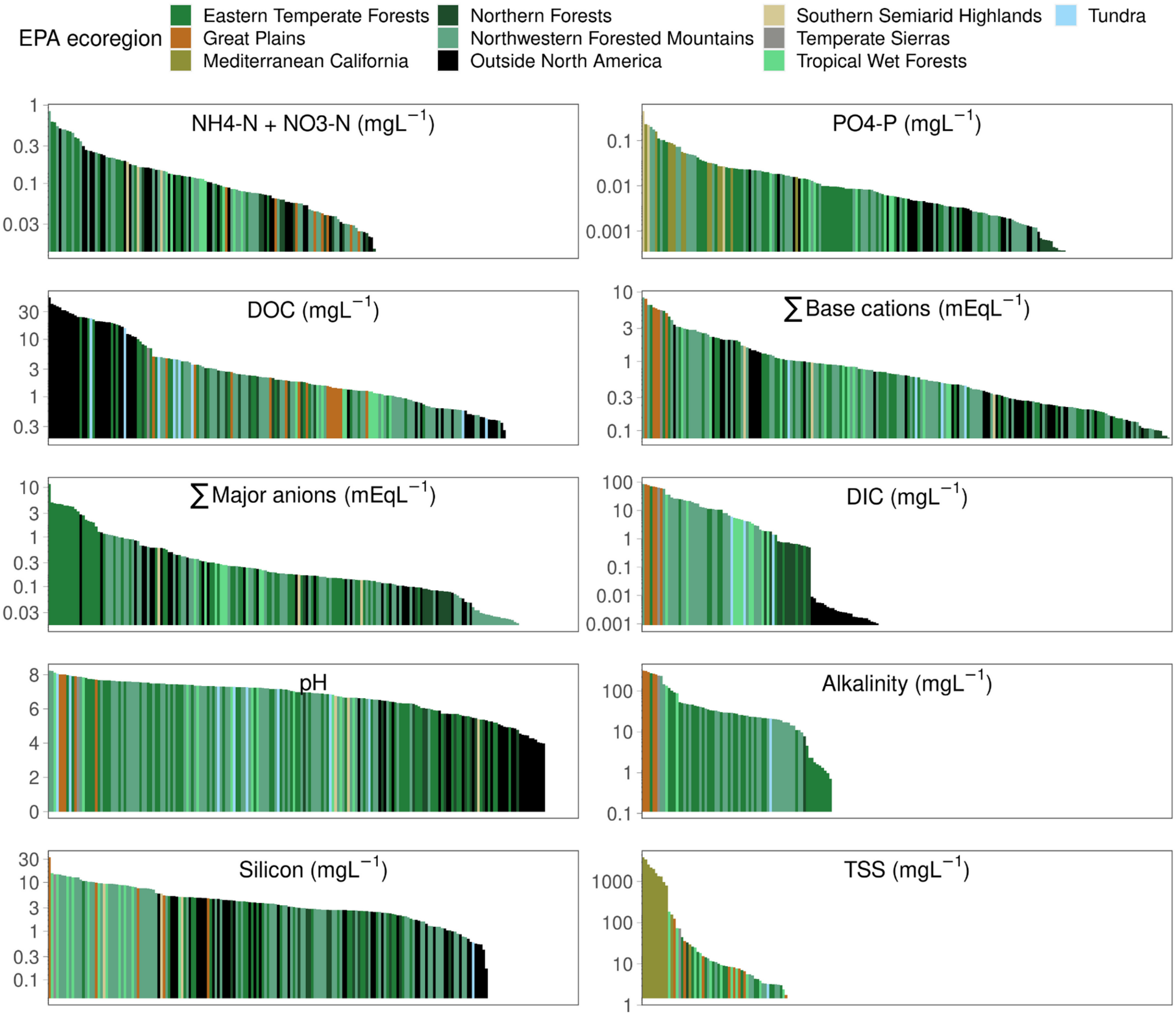


Figure 4. Distributions of chemical properties across MacroSheds sites. Each vertical bar represents a single site. For every panel except “pH”, values are log10 transformed to increase the visibility of the bar colors.

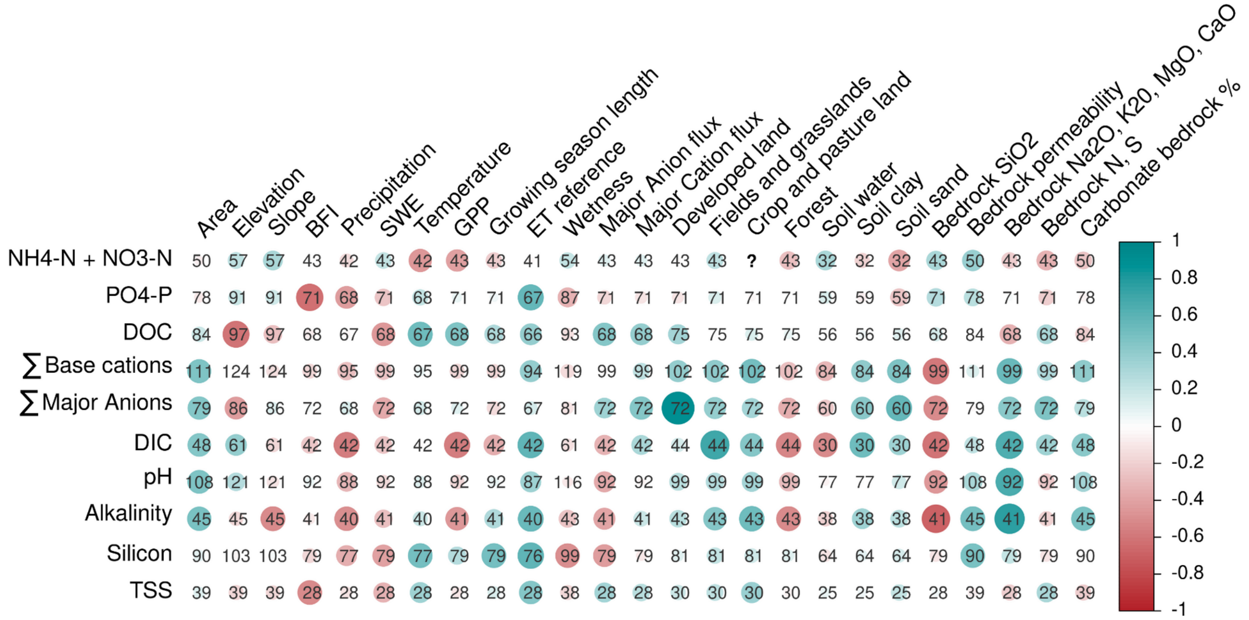


Figure 5. Pearson correlations of watershed attributes with concentrations of major solute categories. Concentrations were computed as mean annual volume-weighted concentration, in equivalents where applicable. Numbers inside each circle represent the number of sites included in the correlation. Records prior to January 1, 2000 were omitted before computing correlations.

Glossary of Terms (*as used in this document)

programmatic: of a computational task, performed with repeatable code, rather than graphical interaction

routine: a programmed operation or set of operations.

pipeline: a series of routines performed on a dataset as it progresses from raw to final form. Each routine may be performed zero or more times during the course of the MacroSheds dataset build process, depending on which components need to be (re)built.

munge: to transform, subset, merge, clean, supplement, or in just about any other way modify data in preparation for analysis, sharing, etc.

harmonize: to munge irregular data structures and formats into a consistent and interoperable unity.

watershed: all land area contributing runoff to a point of interest along a stream, regardless of contributing area. Does not necessarily account for inputs from subsurface flow or human-constructed diversions. The terms “catchment” and “basin” are sometimes used in this way.

*site**: an individual gauging station or stream sampling location and its watershed.

*domain**: one or more sites under common management.

*network**: one or more domains under common funding/leadership.

*product**: a collection of data, possibly including multiple datasets/tables. Primary sources may separate products by temporal extent/interval, scientific category, detection method, and/or sampling location. MacroSheds products are detailed below.

site-product, *site-year*, etc: terms like these are used to designate various subdivisions of the overall MacroSheds dataset. A site-product, for example, is the collection of all data for a single MacroSheds product, available at a single site.

MacroSheds data are organized into the following products:

discharge: streamflow; water volume over time; reported in L/s.

stream chemistry: concentration of chemical constituents in stream water; reported in mg/L or mEq/L.

stream flux: mass of chemical constituents in stream water, per watershed area, over time; reported in kg/ha/d.

precipitation: rainfall, snowfall, or both combined; reported per watershed in mm.

precipitation chemistry: concentration of chemical constituents in precipitation; reported in mg/L or mEq/L; averaged across watershed area.

precipitation flux: mass of chemical constituents in precipitation, per watershed area, over time; reported in kd/ha/d.

watershed attributes: areal watershed summary statistics, describing climate, hydrology, geology, terrain, vegetation, soil, and landcover

Data Description

The MacroSheds dataset and all associated documentation can be found on Figshare, at https://doi.org/10.6084/m9.figshare.c.5621740. This URL will always point to the most recent dataset version, and at the time of this writing is synonymous with https://doi.org/10.6084/m9.figshare.c.5621740.v1. When new versions of MacroSheds are published, the old versions will still be accessible by appending a version number to the end of the base URL in the above fashion.

This dataset is derived from data already published in public repositories, primarily from U.S. federally funded watershed studies, and in compliance with existing grant requirements. The core dataset consists of two components, referred to below as “time series” and “watershed attributes.” Each of these components has a “CAMELS-compliant” counterpart that conforms to the variables and methods used in the CAMELS dataset.

The time-series component is a harmonization of stream discharge, precipitation depth, and almost 200 stream and precipitation variables, including concentrations of major and minor ions, nutrients, metals, photosynthetic pigments, dissolved gases, and more. We also report temperature, turbidity, and other common water quality metrics. The total numbers of sites with discharge and chemistry data are 178 and 481, respectively. The total number with both is 168. For a complete list of variables by site and temporal range, please visit the interactive data catalogs under the Data tab at macrosheds.org. A static table is also available in file 05b_timeseries_variable_metadata.csv of our Documentation on Figshare.

In addition to our core time-series dataset, we provide a separate, supplementary collection of "CAMELS-compliant Daymet forcings" that conforms to the Daymet variables and methods used in the CAMELS dataset (Daymet: Thornton et al. 2020).

The core watershed attributes component is an extensive spatial summary dataset, compiled from published, gridded products. It describes climate, geology, terrain, vegetation and land cover for each watershed in the time-series dataset that has discharge data. We also provide a separate, supplementary collection of "CAMELS-compliant watershed attributes" that conforms to the variables, data sources and methods used in the CAMELS dataset (but see caveats in the "Comparison with Existing Datasets" section below).

MacroSheds time-series data are tiered according to the restrictiveness of licensing and intellectual rights (IR) terms associated with their primary data sources. Data tiers and license/IR information are detailed in our Data Use Agreements (see link_pending_review or 01a_data_use_agreements.docx on Figshare). Citations for all MacroSheds primary sources are included in Tables 1 and 2. A full collection of attribution, contact, and legal information can be found in our documentation on Figshare (see 01b_attribution_and_intellectual_rights_complete.xlsx). Please see the "Data Use and Recommendations for Reuse" section for instructions on efficiently achieving license/IR compliance as a user of MacroSheds data.

MacroSheds time-series data are provided as feather files, data frames serialized and compressed in a language-agnostic format. They are also available in CSV format upon request. Each file contains data for a single site-product, indexed by datetime and variable. For time-series data, the column structure is as follows (hereinafter referred to as "MacroSheds format"):

1. datetime: Date and time in UTC.
2. site_code
3. var: Variable code, including prefix. See “Sampling Methods” subsection below.
4. val: The data value.
5. ms_status: See “Technical Validation” section below.
6. ms_interp: See “Temporal Imputation and Aggregation” subsection below.
7. val_err: The combined standard uncertainty associated with the corresponding data point. See “Detection Limits and Uncertainty” subsection below.

Table 1. MacroSheds time-series data citations, by network and domain.

Network	Domain code	Sites	Citations
LTER	arctic	5	Bowden 2021a-d; Kling 2016a-t; 2019; Shaver 2019; Zarnetske 2020; Zarnetske, Bowden, and Abbot 2020a,b
LTER	baltimore	9	Cary Institute of Ecosystem Studies, Lagrosa, and Welty 2017; Groffman and Martel 2020; Groffman, Rosi, and Martel 2020a,b; Welty and Lagrosa 2020
Bear	bear	2	Patel, Fernandez, et al. 2020a,b
LTER	bonanza	3	Chapin, Ruess, and Bonanza Creek LTER 2014; 2018; Jones, Chapin, et al. 2020; Jones, Hinzman, and Bonanza Creek LTER 2016; Van Cleve, Chapin, et al. 2018
CZO	boulder	4	Anderson 2021; Anderson and Jensen 2021a-c; Anderson and Ragar 2021a-d; Anderson, Rock, and Ragar 2021; Rock and Anderson 2020
CZO	calhoun	1	Foroughi, Cook, et al. 2019; Mallard 2020; 2021; Wang, Shen, and Shahnaz 2021
CZO	catalina_jemez	12	Chorover, Troch, et al. 2021a,b; Litvak and Brooks 2020a,b; McIntosh, Chorover, et al. 2021a,b; Papuga, Compton, et al. 2021; Papuga, Losleben, and Swetish 2021a,b; Troch and Abramson 2019; 2020; 2021; Troch, Abramson, and Jardine 2021; Troch, Broxton, et al. 2020; Troch, Heidbuechel, and Abramson 2019; 2020
DOE	east_river	11	Carroll and Williams 2019; Carroll, Bill, et al. 2019; 2021; Dong, Beutler, et al. 2020a-c; Newcomer and Rogers 2020; Williams, Beutler, Bill, et al. 2020; Williams, Beutler, Brown, et al. 2020
USFS	fernow	9	Edwards and Wood 2011a-c; Edwards Pamela and Wood 2011
LTER	hbef	9	Hubbard Brook Watershed Ecosystem Record (HBWatER) 2021; U.S. Forest Service 2020; 2021
LTER	hjandrews	10	Fredriksen 2019a,b; Johnson, Rothacher, and Wondzell 2020; Rothacher 2017
LTER	konza	4	Blackmore 2020; Blair 2021; Dodds 2019; 2020a,b,c; 2021a-e; Nippert 2021
USFS	krew	8	Hunsaker and Padgett 2019; Hunsaker and Safeeq 2017; 2018
Krycklan	krycklan	15	Laudon, Taberman, et al. 2013
LTER	luquillo	10	Gonzalez 2015; 2017; McDowell 2021a,b; Ramirez 2020; 2021
LTER	mcmurdo	18	Gooseff and McKnight 2021a-q; Lyons 2016a,b; Lyons and Welch 2016; McKnight and Gooseff 2016a-d
LTER	niwot	7	Caine 2019a-c; 2021a-f; Caine and Niwot Ridge LTER 2021a,b; Caine, Morse, and Niwot Ridge LTER 2020a,b; 2021; Morse, Losleben, and Niwot Ridge LTER 2021a-c; Niwot Ridge LTER and

			Caine 2018; Williams 2019; 2021a,b; Williams, Knowles, et al. 2021
LTER	plum	4	Giblin 2013a-d; 2015a,b; 2016; 2017; 2018; 2019; 2020; Hopkinson 2013a-i; Wollheim 2013a-p; 2014a-p; 2016a-l; 2018a-d; 2019a-f; Wollheim and Green 2018a-p; 2019a-i; Wollheim and Plum Island Ecosystems LTER 2019; 2021; Wollheim and Vorosmarty 2014a-f; Wollheim, Hopkinson, and Plum Island Ecosystems LTER 2019
LTER	santa_barbara	12	Santa Barbara Coastal LTER and Melack 2014a-j; 2019a-at; 2020
USFS	santee	4	Amatya and Trettin 2012a,b; 2018; U.S. Forest Service 2011; 2017
CZO	shale_hills	4	Brantley 2019; Li 2018
USFS	suef	4	Fredriksen and Johnson 2017a,b; Jones and Rothacher 2019
USGS	usgs	1	Courtesy of the U.S. Geological Survey
DOE	walker_branch	2	Mulholland and Griffiths 2016a-c

Watershed attribute data are provided as zipped CSV files in two formats, representing different levels of aggregation. At the broadest level, gridded spatial data are summarized to a single value per variable per watershed, and provided as a single file in cartesian (wide) format. However, some watershed attributes are temporally explicit, and our second format preserves the dates associated with each model estimation or satellite pass. The temporally explicit watershed attribute dataset is separated into six categories (climate, hydrology, land cover, parent material, terrain, vegetation), with one file for each. Column structure is as follows:

1. network
2. domain
3. site_code
4. var: Variable code, including prefix. See “Watershed Attributes Retrieval and Processing” subsection below.
5. date: UTC calendar date.
6. val: The data value.
7. pctCellErr: percent of watershed raster cells with missing values. Not currently retrieved for Google Earth Engine products.

Table 2. Watershed attribute datasets included in MacroSheds, and their primary sources. Datasets retrieved from Google Earth Engine, rather than the primary source, are indicated by “GEE”. An asterisk at the end of a row indicates that the corresponding attributes are included in the CAMELS-compliant supplement to the core MacroSheds dataset, but not necessarily in the core dataset itself.

Attribute(s)	**Source**	**Citation**	
evapotranspiration reference	gridMET (GEE)	Abatzoglou 2012	
LAI, fPAR	MODIS (GEE)	Myneni, Knyazikhin, and Park 2015	
NDVI	MODIS (GEE)	Didan 2015	
vegetation cover	MODIS (GEE)	Townshend 2016	
atmospheric chemical fluxes	NADP	NADP Program Office 2022	
landcover classes	NLCD (GEE)	Dewitz 2021	
soil composition and properties	NRCS-gSSURGO	Soil Survey Staff 2022	
SWE, snow depth	NSIDC	Broxton, Zeng, and Dawson 2019	
NPP and GPP	NTSG (GEE)	Robinson et al. 2018	
soil thickness	ORNL DAAC	Pelletier et al. 2016	
wetness	Oxford MAP (GEE)	Weiss et al. 2014	
temperature and precipitation	PRISM (GEE)	Daly et al. 2008	
base flow index	USGS	Wolock 2003	
bedrock composition and properties	USGS	Olson and Hawkins 2014	
climate	Daymet (GEE)	Thornton et al. 2020	*
subsurface permeability, porosity	GLHYMPS	Gleeson 2018	*
geologic classes	GLiM	Hartmann and Moosdorf 2012	*
landcover classes	MODIS (GEE)	Friedl and Sulla-Menashe 2019	*

Users may access MacroSheds data in several ways. The full dataset is available for download at the Figshare URL above, or through the macrosheds package for R (https://github.com/MacroSHEDS/macrosheds; Rhea, Vlah, and Slaughter 2021). It can also be explored using a visualization platform at macrosheds.org. A compendium of MacroSheds variables, sites, sources and associated metadata can be found in our documentation on Figshare. An interactive data catalog is available under the Data tab on macrosheds.org.

Methods

Criteria for Dataset Discovery and Inclusion in MacroSheds

Sites included in MacroSheds were primarily identified through the NSF-funded LTER, LTREB, and CZNet (formerly CZO) programs (112 of 168 sites, as of MacroSheds v1.0). Additional sites funded or managed by the U.S. Geological Survey, Department of Energy, and Forest Service were identified through personal communication, literature search (long*term AND watershed*), or by perusing government websites. The Krycklan Catchment Study in Sweden is currently the only domain within MacroSheds that is not associated with the federal government of the U.S.A., but it will be joined by other U.S. and international watershed studies as the MacroSheds project expands.

To be considered for inclusion in MacroSheds, a site requires: automated monitoring of stream discharge, routine sampling of stream chemistry, at least a full year of each (minus periods of freezing or drying), and public data hosting (with some exceptions). Additional data describing the quantity and chemistry of precipitation are highly valuable, but not required. Watershed boundaries can be delineated and geospatial data gleaned via MacroSheds tools, so are not required.

Data Processing System: Design and Overview

MacroSheds acquires and processes data within a system of serial ingestion pipelines, written entirely in R (R Core Team 2021). Source code is designed functionally and organized hierarchically, so as to emulate the hierarchy of network-domain-site organization across institutions and within the resultant dataset. This allows routines common to arbitrary subsets of sites to be dynamically loaded and called wherever applicable, minimizing code redundancy.

For each domain: discharge, precipitation, and chemistry time series are first downloaded and saved locally in whatever form and format they are provided. They are then munged by site-product into MacroSheds format. If a watershed boundary is not provided, it is delineated. Additional products are then derived, namely stream solute flux and watershed-mean precipitation depth, chemistry, and solute flux. Finally, we generate spatial summary statistics for each watershed.

The processing system is designed insofar as possible to accommodate future deviations from the ways primary sources currently structure and serve their products. Each pipeline is fault-tolerant, so if provider-side changes introduce errors at any stage of data access or processing, the errors are logged, the developers are notified by email, and the system moves on. MacroSheds also uses a custom toolkit for tracking the progress of each pipeline and efficiently (re)generating only components that have changed. At a future stage of the project, the processing system will run on a schedule, automatically rebuilding MacroSheds products as new versions of their precursors are published.

There is no database or warehouse behind the MacroSheds dataset. Reads, writes, and modifications are performed wholesale by site-product, rather than individually by record, which permits each site-product to be serialized and served as a single file. For serialization, we have chosen feather format (Wickham 2019), which facilitates efficient passing of data between R, Python, Julia, and any other language that supports the concept of a “data frame.” MacroSheds data may also be requested in CSV format.

Time-series Data Access and Amenity

Among the 25 domains currently included in MacroSheds, we have identified five distinct tiers of “data amenity”, or the convenience with which we were able to access discharge, precipitation, and chemistry data and harmonize it within a domain. Here, data amenity encompasses the core elements of FAIR principles (Wilkinson et al. 2016), but also whether conceptually adjacent datasets share internal structure, and whether and how revisions are designated. Importantly, data amenity tiers say nothing of the *quality* of a domain's data–only of its data structure and infrastructure. Licensing and intellectual rights restrictions are also a separate issue, with a separate tiering system (see link_pending_review or 01a_data_use_agreements.docx on Figshare). Our data amenity tiers range from A, the most amenable, to E, the least amenable.

At Tier-E, data access is through personal correspondence only. As such, internal file structure is unpredictable and programmatic version-checking is impractical. We have generally avoided Tier-E domains, and make no guarantees about their continued inclusion in MacroSheds, as they require an ongoing time commitment from our developers. We encourage watershed data managers to contribute routinely to public repositories like EDI, HydroShare, or ESS-DIVE, so that we can build automated connections to MacroSheds.

Many datasets are hosted as hyperlinked, static files (Tier-D). This way of serving data is standardized only by the rules of transfer protocols (HTTP, FTP, etc.), which do not facilitate reliable file versioning (Belshe et al.; Postel & Reynolds et al. 1985); however, it is possible to use the last-modified date in the header of a static file as a proxy for file version, as MacroSheds does. Many USFS and DOE domains, and even some CZNet domains, are Tier-D.

By hosting data in any public data repository that follows FAIR data standards, a domain can easily achieve Tier-C data amenity or higher, meaning related files are naturally grouped or linked in a way that aids discovery. Most repositories permit straightforward versioning of files and file collections; however, in Tier-C the onus is on data managers to establish that an uploaded resource is a new version of some existing resource. Most CZNet domains are housed on CUAHSI's HydroShare, a premier environmental data and code repository that allows for easy creation of new versions of "formally published" resources.

However, some CZNet domains have not published their data formally, and edit their existing resources rather than creating official new versions. This makes programmatic identification of new file versions at least as difficult as with Tier-D data amenity.

Datasets associated with Tier-B domains are easily found and fully versioned. Within MacroSheds, most domains associated with the LTER network are Tier-B, owing in part to the strict metadata and publishing requirements of the EDI data portal and underlying PASTA+ repository, which all but ensure proper versioning and within-domain findability of related files. Still, for Tier-B domains, neither data hosting architecture nor management dictate the internal structure of files.

At the forefront (Tier-A) of data amenity are the USGS and NEON domains–each also networks per se–which provide systematic access and consistent data structure across all the sites they manage. This means the URL for e.g. water quality time series at site A is intuitively related to that for site B, and that once downloaded, the two datasets are structured and formatted identically. To boot, NEON and the USGS provide API endpoints by which to interact with their collections programmatically. In R, we conveniently queried these endpoints through official client packages (Lunch et al. 2021; De Cicco et al. 2022). Because Tier-A institutions control data collection, storage, and hosting, they are able to establish a consistency of access and internal structure that is much more difficult to achieve post-hoc.

Please note that high data amenity does not imply high data quality, or even out-of-the-box usability. NEON remains in its early operational phase, and we have identified a large number of water quality and continuous discharge anomalies that require correction or removal from published products (Rhea et al. in review). MacroSheds intends to include NEON data in a future release, pending resolution of these issues.

Time-series Data Processing

This section details major steps taken to harmonize disparate chemistry, discharge, and precipitation data into MacroSheds format (see “Data Description” section above) and extract useful metadata. In any harmonization effort, there is a tradeoff between fidelity to the original datasets as they are, and cohesion of the aggregate set. We have endeavored for a MacroSheds dataset that is parsimonious but high in analytical potential, and that assimilates provided metadata where practical.

Each data ingestion pipeline performs a wide variety of basic munging routines. For a technical account of the steps involved in (1) conforming site and variable names, (2) resolving datetime formats and time zones, (3) converting units, and (4) reshaping data tables, please consult the code documentation included with time-series data at https://doi.org/10.6084/m9.figshare.c.5621740. The rest of this section covers quality control assimilation, metadata extraction, imputation, and uncertainty.

Sampling Methods

The MacroSheds dataset includes measurements recorded by installed equipment and by hand (grab sample), and end users may wish to filter it accordingly. We further distinguish between measurements made via sensors versus analytical or visual means. The former distinction is made programmatically with simple heuristics (e.g. inconsistent sample interval precludes autosampling), and the latter by consulting primary metadata. These distinctions are summarized as two-letter “sample regimen” codes prefixed to each MacroSheds variable code: “I” or “G” for “installed” vs. “grab,” and “S” or “N” for “sensor” vs. “non-sensor.” For example, “IS_discharge.”

At present, we do not report specific analytical methods for time-series variables, effectively assuming that commensurate units imply commensurability. We know this to be misleading for some variables–in particular those measured via fluorescence or absorbance–and intend to include more detailed methods for at least these variables (e.g. FDOM, turbidity) in a future release.

Detection Limits and Uncertainty

We were able to locate published detection limits (DLs) for solute concentrations of only ten of the 24 domains included in version 1 of the MacroSheds dataset. For the rest, we assumed each variable's DL to be the median DL for that variable across the ten domains with reported values. For some domain-variables, multiple DLs were reported, in which case we used the within-domain median when computing the median between domains. We do not attempt to infer DLs from the data, e.g. by assuming they are approximated by the minimum reported absolute value. This risks egregious overestimation wherever measured values never approach the DL, or underestimation wherever reported values have been transformed or determined via a calibration or rating curve.

Below-detection-limit (BDL) measurements are variously reported by primary sources as ½ DL, ¼ DL, DL, 0, missing, etc. For consistency, we replace any value flagged as below-detection-limit (BDL) with ½ of the reported/estimated DL and set the corresponding ms_status to 1 (see the Technical Validation section). For the rare case in which a value is flagged as BDL, and no DL is reported for the corresponding variable at any domain, we set the value to 0 and the ms_status to 1. We emphasize that accurate cumulative flux calculations depend on relatively complete data records. It is thus critical that BDL samples be given a numeric value, so they are not confused with records for which a measurement is truly missing, and must be imputed.

Before MacroSheds performs any mathematical transformation on raw data, uncertainty is attached to each record. Due to the scarcity of reported measurement or analytical precision/uncertainty, we have chosen not to propagate reported values. Instead, initial uncertainty for each domain-variable is determined by $u = 10^{-p}$, where *p* is the precision of the variable's reported DL, after conversion to

MacroSheds standard units. For example, a DL of 0.008 mg/L has a precision of 3 (digits after the decimal), resulting in initial uncertainty of 0.001 mg/L. For domains that do not report DLs, we set the initial uncertainty for each variable according to the minimum (coarsest) reported *p* across all domains that do report DLs. For some variables, we have no basis by which to infer initial uncertainty, so we report it as missing. The two exceptions are discharge and precipitation, both required for computing solute flux. For these, we set initial uncertainty to zero. Uncertainty is then propagated through all MacroSheds mathematical transformations via the errors package (Ucar, Pebesma, and Azcorra 2018). A table of all known detection limits and starting precision values can be found in our documentation on Figshare (05f_detection_limits_and_precision.csv).

Temporal Imputation and Aggregation

MacroSheds currently reports all time series (not including temporally explicit spatial summary data) at a daily interval. The timestamp associated with each incoming record is floored to midnight (0 hours, 0 minutes, 0 seconds), and series with a sub-daily interval are aggregated across each 24-hour span. Precipitation, which is reported in mm, is aggregated by sum, while discharge and chemistry are aggregated by mean. After aggregation, any implicit missing values are made explicit, so that there are no missing timestamps within a series. Linear interpolation is then used to fill gaps of no more than three days in each discharge and precipitation series, and no more than 15 days in each chemistry series. In the case of flux series provided by primary sources, the maximum gap length filled is also 15 days. No extrapolation is performed. Records interpolated by MacroSheds are given an ms_interp value of 1; otherwise 0.

Watershed Attributes Retrieval and Processing:

The MacroSheds dataset includes over 60 watershed attributes–spatial summary statistics that may act as drivers of ecohydrological processes. These attributes are derived from modeled and remotely sensed gridded data products from various platforms. Attributes were chosen to capture the range of physical and biological variation seen in natural watersheds, and to allow comparison with other large scale catchment datasets such as StreamCat and CAMELS (see the "Comparison with existing datasets" section below).

Attributes are organized into six categories: vegetation, climate, terrain, parent material, landcover, and hydrology. Every spatial variable in MacroSheds has a two letter prefix to indicate first the variable category, and second the data source. For example, Leaf Area Index (LAI) variables from the MODIS satellite have a prefix of "v" to indicate the vegetation category and a "b" the data source as MODIS, so the median LAI for a watershed has the name "vb_lai_median" in the MacroSheds system.

Gridded products are summarized to watershed boundaries using one of two methods, based on where the source data product is held. For data accessible through Google Earth Engine (GEE), we used the R package "rgee" (Gorelick et al. 2017; Aybar 2021). First watershed boundaries are uploaded to GEE and stored as an asset. Then median and standard deviation values for each watershed at each reported time-step are summarized using the rgee function "reduceRegions." For products not housed on GEE, gridded data are locally processed using the "terra" package for R (Hijmans 2021). A list of gridded data products and their sources is in Table 2.

Most watershed attributes included in MacroSheds are temporally explicit, with sampling/modeling intervals varying from daily to decadal. MacroSheds provides all watershed attributes in their native (as reported by primary source) temporal intervals, and a subset of attributes as averages by site. MacroSheds does not provide all watershed attributes for all sites, as some gridded products are only available for the contiguous USA.

Derivation of Additional Products

The central aim of the MacroSheds project is to engage continental-scale questions about whole-watershed chemical and hydrologic flux. Toward this end, a spatially explicit measure of both influx and outflux is needed. Such a measure requires information not consistently provided alongside the time-series data described above, namely watershed-mean precipitation and precipitation chemistry, and the watershed boundaries needed to compute them. Methods for calculating flux are many, so we employ a single method across all MacroSheds sites, though we also report some flux products as calculated by primary sources. We do not yet officially publish MacroSheds flux estimates, but they can be easily computed via the macrosheds R package.

Watershed Delineation

For any watershed boundary not provided as a georeferenced spatial file, MacroSheds performs a delineation from the point of the stream gauge or sampling site (pour point). This process cannot be reliably automated, due in part to imperfections in digital elevation models (DEMs), and in part to the fact that stream site locations are usually recorded from the banks nearby. Sometimes the watershed “found” by a delineation algorithm is actually a subset of, or adjacent to, the target watershed, and only visual inspection reveals the error. We rely on a semi-automated, interactive approach that delineates one or more candidate watersheds for each site, starting from one or more unique pour points. DEMs are retrieved using the “elevatr” package (Hollister et al. 2020) for R, and iteratively expanded any time a proceeding delineation meets the DEM edge. Candidate watersheds are presented for visual inspection and topographic comparison via package “mapview” (Appelhans et al. 2021). Hydrologic conditioning, pour point snapping, and delineation leverage package “whitebox” (Wu 2021). If none of the candidates appears to represent the target watershed, the process can be conveniently repeated using updated parameters. For a detailed discussion of these, see the macrosheds R package documentation.

Spatial Interpolation of Precipitation Data

Each MacroSheds watershed is rasterized, or gridded, from the DEM used during delineation, or from one so retrieved. Precipitation chemistry is then imputed to each cell of the watershed raster by inverse squared-distance weighted interpolation (IDW; Shepard 1968), using information from all precipitation gauges associated with the domain. Watershed-mean precipitation chemistry is then computed as the mean across all raster cells, separately for each solute and each day with data.

Due to the orographic effect in mountainous regions, precipitation depth at a given elevation can be estimated from a local, linear relationship (Hevesi et al. 1992). Daily precipitation depth in the MacroSheds dataset is computed as a simple equal-weight ensemble of two predictions, one generated by IDW and the other from the empirical elevation-precipitation relationship among all domain-associated gauges. On days for which fewer than three gauges are in operation, only the IDW prediction is used.

Flux Calculation

In a future version of the MacroSheds dataset, we will include solute flux directly. For now, we provide discharge, precipitation, and concentration data, and let end-users compute flux or volume-weighted concentration (VWC) via the macrosheds R package, using the `ms_calc_flux` function. Solute flux is computed according to equations 1 and 2,

(1) $$F_s = \frac{Q C_s}{A}$$

(2) $$F_p = P C_p$$

where F_s and F_p are solute flux in stream water and precipitation, Q is discharge, P is average precipitation depth over the watershed, C is solute concentration, and A is watershed area. F is reported in kg/ha/d, and is calculated on each day for which Q or P, and corresponding C, are measured or interpolated. If ms_status or ms_interp are equal to 1 for either factor, resulting F inherits the same.

VWC is computed according to equation 3,

$$(3) \qquad \mathrm{VWC} = \frac{\sum_{i=1}^{N} C_i \cdot V_i}{\sum_{i=1}^{N} V_i}$$

where N is the number of days in the aggregation period (e.g. a month or a year), C is solute concentration, and V is daily volume of streamflow or precipitation.

Technical Validation

Quality control (QC) practices in watershed ecosystem science are almost as diverse as watersheds themselves; however, there are common currents that run through every data flag and comment. For example, if a sensor is buried in sediment for a week, that week's data should be omitted from analyses. Likewise with a sensor that is wildly malfunctioning or a water sample that is severely contaminated. Ultimately, when data are analyzed, each record is included, omitted, or included with caution. Thus, we have distilled each domain's data flags and comments down to either "bad data", which is excised during munging, "questionable", or "clean." If a flag definition or comment makes any mention of insufficient sample volume, minor contamination, sensor drift, or some other condition that *could*, but does not necessarily, invalidate the corresponding record, we designate it "questionable," and set its ms_status value to 1. Only if flags and comments are absent, or specify no issues of potential concern, do we designate a record “clean,” and set its ms_status to 0. The documentation files included with time-series data downloads can be used to locate the specific URLs and access dates of original data and metadata, where fully detailed flag information can be found.

We do not report BDL samples as such, but instead assign them an ms_status of 1. We then report all detection limits–either given by primary sources or estimated by MacroSheds–in our documentation on Figshare (see 05f_detection_limits) so that BDL status can be reconstructed if necessary. For more on how MacroSheds handles detection limits, see the “Detection Limits and Uncertainty” subsection above.

MacroSheds currently performs minimal QC beyond assimilating primary source flags and comments; however, we do filter each time-series record through a very loose “range check,” intended to ensure that physically impossible values that happen to have evaded primary source QC are omitted from our aggregate dataset. Minimum and maximum reasonable values have been chosen so as not to risk any encroachment on the true natural range for each variable. A full list of these filter ranges can be found in 05e_range_check_limits.csv in our dataset documentation on Figshare. Beyond range checking, we currently rely on the expertise of primary data providers to publish data that has been vetted. We intend to implement more sophisticated anomaly detection in a subsequent release of the MacroSheds dataset and portal.

Some datasets were excluded from this synthesis due to concerns about the quality of the required solute chemistry and hydrology datasets. All of the aquatic sites within NEON are currently excluded on this basis, though we intend to include NEON sites in a future version of MacroSheds (Rhea et al. in review).

Data Use and Recommendations for Reuse

The MacroSheds dataset is intended to provide analytical material for diverse investigations of watershed form and function. It is especially suited to comparing watersheds in terms of inputs and outputs of energy and material. In addition to precipitation, solute chemistry, and streamflow time-series data, it contains a comprehensive set of potentially predictive watershed attributes for each of 178 stream monitoring sites. To our knowledge, the MacroSheds dataset is the most comprehensive analysis-ready collection of watershed biogeochemical data for North America (but see Sterle et al. in review).

MacroSheds can also be used as a small-watershed supplement to hydrological datasets like CAMELS and GAGES-II. See the next section for a detailed comparison.

Because MacroSheds time-series data are currently represented at daily intervals, this dataset is *not* well suited to sub-daily analyses, such as those focused on stormflow dynamics. A future version of MacroSheds may include time-series data at 15-minute resolution.

To meet acceptable use requirements of the MacroSheds dataset, one must comply with the licensing and intellectual rights (IR) stipulations of all applicable primary sources. We have created two convenient resources to help end-users achieve acceptable use. The first, for users of the `macrosheds` R package, is the `ms_generate_attribution` function, which produces a list of acknowledgements, citations, contact emails, and IR notifications based on a given `data.frame` in MacroSheds format. The second is a document included with our dataset documentation on Figshare (01b_attribution_and_intellectual_rights_complete.docx) that contains essentially the output of the `ms_generate_attribution` function, assuming the entire MacroSheds dataset is being used. The content of this document can be copied and pasted, in whole or in part, depending on how much of the overall dataset is actually used. Domain-specific subsets of this document are included alongside downloaded time-series data.

A summary of IR stipulations by primary source is provided in section 4.1 of our Data Use Agreements (see link_pending_review or 01a_data_use_agreements.docx on Figshare), and a complete accounting of licenses, IR, contact information, DOIs, and more can be found in 01b_attribution_and_intellectual_rights_complete.xlsx.

Comparison with Existing Datasets

The subset of MacroSheds that relates to streamflow and climate forcings makes it a valuable supplement to existing datasets like CAMELS (671 sites) and GAGES-II (9067 sites). Using CAMELS methods, we have compiled watershed attributes and Daymet forcings, for each MacroSheds site, that are immediately commensurable with the published CAMELS dataset, enhancing the predictive power of the combined set, especially for small watersheds. Of the 178 sites with discharge data that MacroSheds adds to this corpus, 122 have watershed areas of 10 km^2 or less, and 68 have areas of 1 km^2 or less. For CAMELS, these numbers are 8 and 0, respectively. For GAGES-II, they are 207 and 2 (Figure 2).

Please note that we used gSSURGO (Soil Survey Staff 2022) instead of the superseded STATSGO dataset for soil characteristics. Two other CAMELS watershed attributes, pet_mean and aridity, were also computed differently for MacroSheds watersheds. For these, we solved the Priestly-Taylor formulation by using a gridded product (Aschonitis et al. 2017), rather than calibrating ourselves.

In addition to the original U.S.-based CAMELS dataset, there are now equivalent products for Chile (Alvarez-Garreton et al. 2018), Great Britain (Coxon et al. 2020) and Brazil (Chagas et al. 2020). As of this writing, there is also a soon-to-be-published CAMELS-Chem dataset, which supplements 506 of the original CAMELS sites with measurements of 18 common stream chemistry constituents (Sterle et al. in review). There are also many networks of watershed ecosystem observatories with varying degrees of internal data consistency, and which ultimately we hope to coalesce into a more international MacroSheds. These include ECN (UK; Lane 1997), SAEON (South Africa; Van Jaarsveld, et al. 2007), CERN (China; Fu et al. 2010), TERENO (Germany; Zacharias et al. 2011), TERN (Australia; Karan et al. 2016), OZCAR (France; Giallardet et al. 2018), eLTER (Europe; Mollenhauer et al. 2018), and ILTER (global; Mirtl et al. 2018).

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Bear Brook (Maine)
CZNet: Boulder Creek, Calhoun, Catalina-Jemez, Susquehanna Shale Hills
USDOE: East River, Walker Branch
Krycklan Catchment Study
LTER: Arctic, Baltimore Ecosystem Study, Bonanza Creek, Hubbard Brook Experimental Forest, H. J. Andrews Experimental Forest, Konza Prairie, Luquillo, McMurdo Dry Valleys, Niwot Ridge, Plum Island Ecosystems, Santa Barbara Coastal
NEON
USFS: Fernow, King's River, Santee, and South Umpqua Experimental Forests/Watersheds
USGS

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