popler: An R package for synthesis of population time series from long-term ecological research

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Running headline: The popler database and R package

[Tom's comments appear in red italics.] *[Aldo's comments appear in blue italics.]*

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Abstract

1. Population dynamics play a central role in the historical and current development of fundamental and applied ecological science. The nascent culture of open data promises to increase the value of population dynamics studies to the field of ecology. However, synthesis of population data is constrained by the difficulty in identifying relevant datasets, by the heterogeneity of available data, and by access to raw (as opposed to aggregated or derived) observations.

2. To obviate these issues, we built a relational database, `popler`, and its `R` client, library("popler"). `popler` accommodates the vast majority of population data under a common structure, and without the need for aggregating raw observations. library("popler") is designed for users unfamiliar with the structure of the database and with the SQL language. This `R` library allows users to identify, download, explore, and cite datasets salient to their needs.

3. We implemented popler as a PostgreSQL instance, where we stored population data originated by the United Stated Long Term Ecological Research (LTER) Network. Our focus on the US LTER data aims to leverage the untapped potential of this vast open data resource. The database currently contains 272 datasets from 25 LTER sites and is poised to grow to accommodate forthcoming LTER data as well as non-LTER studies.

4. The combination of the online database and the `R` library("popler") is a resource for data synthesis efforts in population ecology. The common structure of `popler` simplifies comparative analyses, and the availability of raw data confers flexibility in data analysis. library("popler") maximizes these opportunities by providing a user-friendly interface to the online database.

Keywords

open long-term population data, US Long Term Ecological Research Network data, online database, database structure, PostgreSQL, R package, data synthesis, comparative analysis

Introduction

Population dynamics – changes in species' abundance and composition through time and space – are central to ecology for both applied and fundamental reasons. Populations are the building blocks of ecological dynamics at higher scales of organization, and examples abound showing how the study of population ecology improves understanding in evolution (Metcalf and Pavard, 2007), community ecology (Levine and HilleRisLambers, 2009), and ecosystem ecology (Medvigy et al., 2009; Fisher et al., 2018). Given their central role, studies of population dynamics will be an essential component in the advances allowed by the flourishing culture of open access and data synthesis.

The increase in freely available data is poised to change ecological science (Laurance et al., 2016). The rising focus on open data is clear in changing publishing standards, in the design of observational networks (Schimel et al., 2007), and in the availability of previously proprietary data (Kratz et al., 2003; Bechtold et al., 2005). This deluge of open data holds promise to facilitate comparative analyses and to test the generality of ecological hypotheses. For population dynamics in particular, it is the increasing availability of long-term data that will likely yield the most substantial scientific advances, as long time series are required to detect trends in abundance (Lindenmayer et al., 2012), quantify temporal variance (Compagnoni et al., 2016), and identify endogenous (Knape and de Valpine, 2012) or exogenous (Hampton et al., 2013) drivers of population fluctuations.

To our knowledge, there is currently just one publicly accessible database focused on long-term population dynamics: the Global Population Dynamics Database (GPDD, Inchausti and Halley, 2001). The GPDD provides over 5000 time series of population size longer than 10 years for over 1800 animal species. This database has been powerfully leveraged for comparative analyses and syntheses (e.g., Knape and de Valpine, 2012) but it has some important limitations. GPDD time series are not spatially replicated – there is one observation of population size or density for each temporal replicate, with no estimate of uncertainty – making it difficult or impossible to isolate different sources of variability. Additionally, the GPDD focuses on single species dynamics, making it difficult or impossible to link the dynamics of multiple fluctuating populations within communities.

One of the best sources of publicly available long-term data is the Long-Term Ecological Research (LTER) network. The LTER was founded in 1980 and grew from the original six sites to the current 28 sites throughout North America plus one each in Puerto Rico and Antarctica. Synthetic and comparative studies from the LTER network have made valuable contributions to ecological understanding (Knapp et al., 2012). However, the majority of LTER synthesis research has focused on ecological dynamics at the community (e.g. Wilcox et al. (2017)) and ecosystem (e.g. Knapp and Smith (2001)) scales. Nevertheless, every LTER site collects population abundance data as one of its five core areas of continuous observations (Callahan, 1984). These population time series include both single- and multi-species studies. In our opinion, these data, which have been accumulating since 1980, are under-used.

One issue that may limit the use of LTER population data in synthetic, comparative studies is their heterogeneity. The structure of LTER data sets may be widely different, employing a variety of data types (counts of individuals, biomass estimates, percent cover, etc.), experimental designs driven by the priorities of particular PIs, and diverse replication schemes – idiosyncrasies that may be difficult to accommodate in a one-size-fits-all database. However, these challenges also present valuable opportunities. For example, the hierarchical replication structure of many LTER studies (e.g., subplots within plots within transects) can facilitate more sophisticated statistical investigation than would be possible with simpler, aggregated, or unreplicated data.

To overcome the issues posed by heterogeneous data structures, we developed `popler` (POPulation dynamics in Long-term Ecological Research), an online database of LTER population studies. We also developed a companion R package to aid in discovery, querying, and synthesis. The `popler` database defines a common data structure to facilitate the identification, access, and manipulation of raw and heterogeneous population data through a user-friendly R package. Our goals here are to provide introductions to the database and package. Our focus here is on LTER time series but our database schema can, in principle, accommodate any population dynamics dataset; expanding `popler` beyond the LTER network is a priority for future development.

The **`popler`** database

To combine population data from the LTER network using a common structure, we identified a set of relevant variables (Table 1) and organized them into a relational database (Fig. 1). We store "raw" data, warts and all, meaning that we have not modified, edited, or aggregated the original observations.

For inclusion in `popler`, we only considered studies that included (1) repeated observations of populations or individuals through time, (2) at least five years of data (as of database creation in 2017), and (3) taxonomic information associated with abundance observations (e.g., we excluded time series of functional groups). We provide technical details of database creation in Appendix S1.

The `popler` database currently contains data from 272 studies (272 of which are experimental) representing 3547 cumulative years of observations with a mean study duration of 13.04 years. `popler` contains data from 691 plant species, 349 animal species, and 1 fungal species.

Population data

We define "population data" as time-series of observations on the size or density of a population of a species or other taxonomic unit. Observations of population size are stored in a variable called `abundance_observation` and can be measured as a count, biomass, density, or cover. These four types of population data are stored in the homonymous tables of the database (Fig. 1A).

The population datasets contained in popler are always replicated temporally. Temporal replicates are identified with up to three variables: `year`, `month`, and `day`. Population data are also almost always spatially replicated, and spatial replicates are often nested, where for example a study might include separate sites, each of which contains intermediate spatial replicates (e.g. a transect, a block), which in turn contain the smallest spatial replicate at which observations are made (e.g. a plot, a quadrat). The hypothetical study described above would have three nested levels of spatial replication, identified by three numbered `spatial_replication` variables. In `popler`, we accommodate data sets with up to five spatial replication levels (Table 1). We call the first and therefore largest spatial replicate "study site" (Fig. 1C). Note that this does not refer to the LTER site, one of the 28 NSF-supported locations (Table S3).

popler contains both observational and experimental studies. Experimental datasets contain information on one or more experimental treatments. Popler accommodates information on up to three experimental treatments, identified by three numbered treatment_type variables (Table 1).

Most datasets contain one or more variables in addition to the ones described above which we store in a list of variable called covariates. Covariates can be useful for time series that contain information on population structure *[Did you decide whether / how this would be indicated in the metadata?]*. In these datasets, observations on population size are grouped based on subdivisions of the entire population, such as males and females, large and small individuals, etc.

Finally, in addition to time series of abundance, popler contains individual-level data. This data provides information on the attributes of the individuals, or a subset thereof, that make up a population. We store this information in a dedicated table (”Individual”, Fig. 1A). As individual attributes we consider variables that describe identity, size, sex, life stage or status (e.g. reproductive or non-reproductive). We refer to these individual attributes with the term “structure”: popler accommodates data sets that measure up to four types of structure simultaneously. We store these data in up to four numbered structure_type variables. While these data are not population time series, we chose to include them in popler because they provide information on demographic transitions that can be used to derive estimates of population growth. Moreover, in the cases of datasets that sample all of the individuals in a population, individuals can be aggregated (i.e. summed) as a measure of population size.

Taxonomic information

Each observation corresponds to a taxonomic unit (Fig. 1B),typically a species or a genus but we also include data that refer to a higher taxonomic rank, such as family, or order. popler provides 15 taxonomic ranks, and two additional variables that refer to how taxonomic information is recorded in the original datasets. The additional variables are sppcode, which are taxon-specific alphanumeric codes, and common_name, the common name of each taxonomic unit (Table S1).

popler stores the taxonomic information linked to each study in two tables: one containing the original taxonomic information, the other containing the accepted taxonomic information derived from the former (Fig. 1B). Raw taxonomic data typically contains ambiguities derived by the dynamic changes in species classifications (Chamberlain and Szöcs, 2013). The raw data also typically fail to include higher-level taxonomic information above the genus level. To provide as much taxonomic information as possible, `popler` provides a second table linking taxonomic units provided by the authors to accepted taxonomic units according to the algorithms provided by the R package `taxize` (Chamberlain and Szöcs, 2013). *[Just want to confirm that we are definitely doing this??]*

Study site

We stored the locations of datasets by recording the latitude (`lat_study_site`) and longitude (`lng_study_site`) of study sites (Fig. 1C). Storing this information in a separate table allows for explicit connections between independent data sets collected at the same locations within LTER sites.

Metadata

The metadata table (Table S2 *[Confusing because this table does not have 48 variables]*) provides information on temporal and spatial replication and study design (Fig. 1D), including title, link to online metadata, contact information for data originators, and the type of data provided by the dataset (i.e., which of the five tables in Fig. 1A the data is stored in). All remaining metadata is related to the variables stored in the tables of 1A and 1B. First, we providethe years elapsed between the first and last observation (`duration_years`), and the sampling frequency (`samplefreq`). Second, we provide the number of levels of nested spatial replicates, and with the number of replicates for each spatially nested level. Third, we show whether studies focus on a single species or on multiple species through the `community` variable. Fourth, we identify studies as observational or experimental (`studytype`). If a study is experimental, we provide information on the type of treatments imposed by the study (`treatment_type_n`) and, when available, which one is the control treatment (`control_group`). Finally, when abundance data stored in the `abundance_observation` variable is aggregated across space or time, rather than raw, we consider these data as derived (`derived`).

The `popler` package

The `popler` `R` package consists of three core functions that allow users to browse and retrieve data from the database (Fig. 2). In order of intended use, these functions are: `pplr_dictionary()`, `pplr_browse()`, and `pplr_get_data()` *[I would be in favor of adding the 'o' and 'e' to make it 'popler_browse()' etc.]*.

The `pplr_dictionary()` function

The dictionary function is a good place for new users to begin working with `popler` (Fig. 2). With no arguments provided, this function returns a subset of the most useful metadata variables associated with each dataset (Fig. 1). Providing argument `full_tbl = TRUE` returns all 76 metadata variables. Each one of these variable names can be provided as an argument to `pplr_dictionary()`, which then returns the possible unique values of the variable. For example, `pplr_dictionary(lterid)` returns the three letter codes of the LTER network sites included in `popler`. For numeric variables such as `duration_years`, `pplr_dictionary()` returns a summary including quantiles, mean, and median.

The `pplr_browse()` function

Once the user is familiar with the meaning and content of the variables that define `popler` datasets, they are ready to dig deeper using `pplr_browse()` (Fig. 2). Running `pplr_browse()` without arguments provides the metadata from the entire contents of the database. This will be a $272 * 19$ data frame, with each row corresponding to a study and each column corresponding to a variable defined by `pplr_dictionary()`.

The full strength of `pplr_browse()` is achieved by subsetting studies according to desired criteria using logical expressions. For example, the user might want to consider only studies whose duration is 30 years or greater, which can be subsetted with:

```
LTER_30 <- pplr_browse( duration_years > 29)
```

This operation will create the object LTER_30, which provides metadata for the data sets that satisfy the specified criterion. Multiple criteria may be combined. For example, 30+ year studies of plants can be browsed with

```
LTER_30_plants <- pplr_browse( duration_years > 29 &
                               kingdom == "Plantae")
```

To facilitate data exploration, pplr_browse() output can be printed in a more readable settings by providing report = TRUE as an argument, which opens up a formatted html document. The metadata provided by pplr_browse() not only contains information on the characteristics of a study but also information on how to cite the study, its unique identifiers, including digital object identifier (DOI), and the contact information of study PIs.

The pplr_get_data() function

Once data sets of interest have been identified, pplr_get_data() downloads the data from a server that hosts the database. This function can take as its first argument a browse object, a logical expression, either or both. The data downloaded from popler are in "long" form, meaning that each row of data reports a single measure of population size, and separate variables indicate the temporal and spatial replicate, taxa, etc. This format makes it easy to further subset downloaded datasets with the aim of visualization and analysis.

Ancillary functions

popler also provides three additional functions to open the url of the original dataset, unpack covariates, and provide a citation for each dataset. First, the function metadata_url() launches the online study description in a web browser. Second, the cov_unpack() function extracts a new data including all covariates (which pplr_get_data() does not provide by default). Third, pplr_citation() generates a citation for the originators or each data set.

Limitations and opportunities for development

Working with raw, spatially replicated, and non-aggregated data provides key advantages in quantitative analyses of population dynamics, and these advantages were a driving force behind the development of `popler`. However, users need to examine individual datasets and the associated online study descriptions to understand their peculiarities. Single datasets have unique idiosyncrasies that require vetting. For example, many datasets have gaps or changes in the sampling design during the length of the study, or the `covariates` variable can hold key information. Hence, we urge authors to consult the online documentation of the original datasets.

In the future, there are opportunities to increase the size of `popler` and expand its scope. First, because many of the studies included in `popler` are ongoing, there will be opportunities to run regular updates aimed at including new observations in `popler`. Second, because our schema (Fig. 1) is very general, the database could be expanded to include population datasets outside of the LTER network. Third, it would be valuable to explicitly associate `popler`'s population-level data with environmental drivers, especially climate. It is our intention and hope that the resources provided by `popler` will advance ecological understanding of population dynamics within the LTER network, and more generally.

Acknowledgements

We thank Trevor Drees and Michael Saucedo for assistance in database development. Support for database and package development was provided by the US National Science Foundation to TEXM (DEB-1543651). This research was additionally supported by a Julian Huxley Faculty Fellowship from Rice University and a Faculty Research Grant awarded by the Committee on Research from the University of California, Santa Cruz (KZ). The LTER network is supported by the US National Science Foundation.

Authors' contributions

AC, AB, KZ, MO, TEXM designed and built the database. AC AB, KZ, BD, SM, and TEXM designed and built the R package. AC and TEXM led the writing of the manuscript. All authors contributed to manuscript drafts and gave final approval for publication.

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Table 1: Variables used to store population or individual data in `popler`.

Variable	Description
`abundance_observation`	Measure of population abundance at a specific time and location. This variable measures abundance as a count, biomass, density, or cover. For individual data sets this variable is always equal to 1, because each attribute or set of attributes refer to a single individual.
`day`	Day of observation
`month`	Month of observation
`year`	Year of observation
`spatial_replicate_n`	The n^{th} level of spatial replication, where `spatial_replicate_1` is the study site. `popler` accommodates up to five levels of spatial replication.
`treatment_type_n`	For datasets originating from an experimental study, the n^{th} treatment. `popler` popler accommodates up to three treatments.
`covariates`	Ancillary observations that do not fall into the standard schema of `popler`.
`structure_type_n`	For individual data, these variables measure the n^{th} attribute of individuals (identity, size, sex, status, stage). `popler` accommodates up to four structure types per dataset.

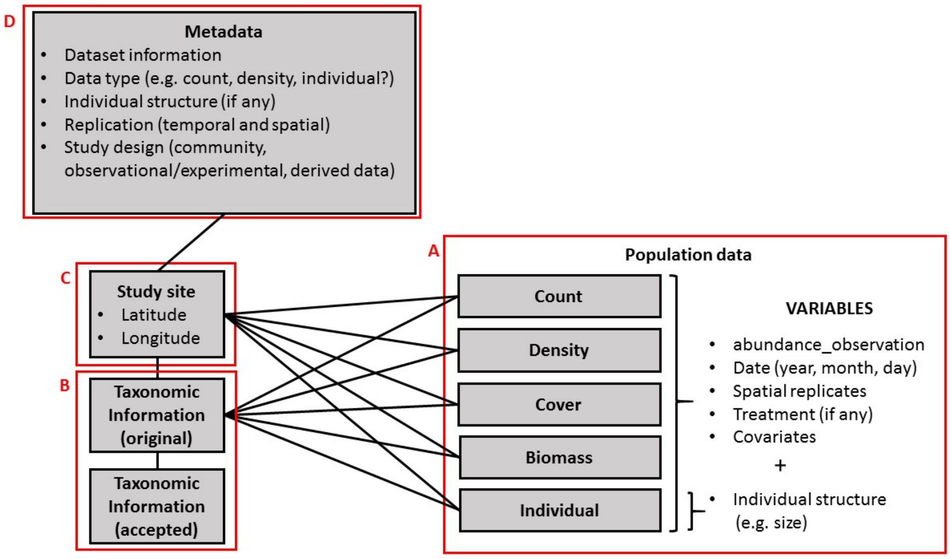
D
Metadata
• Dataset information
• Data type (e.g. count, density, individual?)
• Individual structure (if any)
• Replication (temporal and spatial)
• Study design (community, observational/experimental, derived data)
C
Study site
• Latitude
• Longitude
B
Taxonomic Information (original)
Taxonomic Information (accepted)
A
Population data
Count
Density
Cover
Biomass
Individual
VARIABLES
• abundance_observation
• Date (year, month, day)
• Spatial replicates
• Treatment (if any)
• Covariates
+
• Individual structure (e.g. size)

Figure 1: Schematic representation of the entity relationship diagram of the `popler` database. `popler` provides metadata on the studies that originated abundance data points (D). This metadata contains information on the unique identifiers of each study, on its design (observational or experimental), temporal and spatial replication. `popler` stores the latitude and longitude of the study site (C). Each abundance data point corresponds to a specific taxonomic unit (B). Finally, the time series of population data collected in a study can be of four different types (count, density, biomass, cover), or they may be individual data with attributes such as size or sex (A).*[Replace 'individual structure' with 'individual attribute'.]*

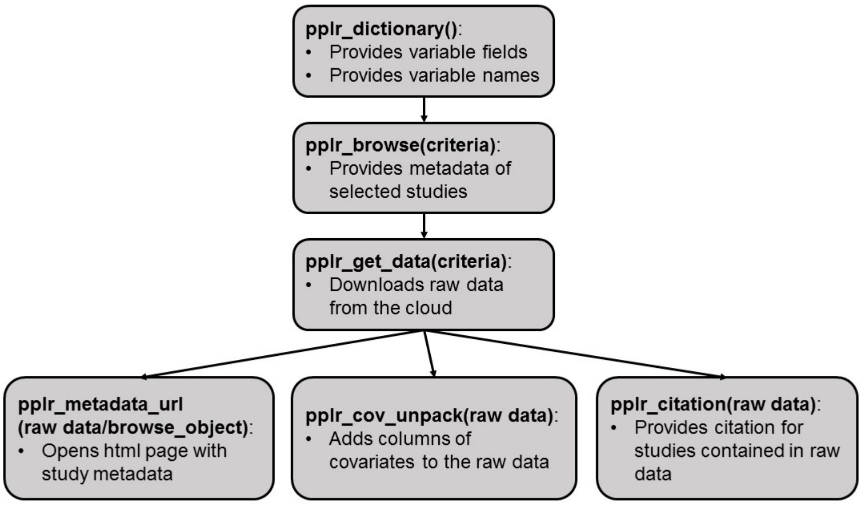
pplr_dictionary():
• Provides variable fields
• Provides variable names
pplr_browse(criteria):
• Provides metadata of selected studies
pplr_get_data(criteria):
• Downloads raw data from the cloud
pplr_metadata_url (raw data/browse_object):
• Opens html page with study metadata
pplr_cov_unpack(raw data):
• Adds columns of covariates to the raw data
pplr_citation(raw data):
• Provides citation for studies contained in raw data

Figure 2: Suggested workflow when using the `popler` R package to interface with the homonymous online database. The function `pplr_dictionary()` refers to the variables of the metadata that describe the data sets contained in `popler`. `pplr_dictionary()` describes these variables and returns their possible values. This information advises which criteria to use when subsetting `popler`. The user can provide a criterion (that is, a logical statement) to browse the metadata, using `pplr_browse()`, or to download data using `pplr_get_data()`. Moreover, the output of `pplr_get_data()` (a data frame) can be the argument of three ancillary functions: `pplr_metadata_url()` opens the webpage containing the original dataset and their associated online metadata. `pplr_cov_unpack()` can be used to format the covariates contained in a raw data object into separate columns of a data frame. Finally, `pplr_citation()` provides a citation for the downloaded data set(s).*[I think it would be simpler to cut the fake arguments from the functions in the figure and just show them with no arguments.]*

Appendix S1: Pre-processing popler data

Before uploading datasets into the online popler database, we combined datasets, transformed datasets from wide to long form, converted non-ASCII characters, and modified ambiguous study site names.

The variables of many datasets were contained in two or more separate files, which we combined in a single file. When the original dataset provided data in wide form, we transformed it into long form. In wide form datasets, abundance data associated with different species was stored in separate columns. popler stores these datasets in long form, whereby each row of abundance data is related to a specific taxonomic unit in the table containing taxonomic information (Fig. 1B). We converted all data in ASCII format, because the encoding of the database is the UTF-8. We often re-defined study site names to unambiguously associate them with one of the 26 LTER sites. Many site names are alphanumeric codes (e.g. "U1") which can overlap across several LTER sites. Hence, we changed site names following a standard formula (namely, from "U1" to "site_sbc_U1", where "sbc" refers to the Santa Barbara coastal LTER site).

In a handful of cases, we removed single data rows from the original dataset. These data rows were associated with two types of typos in the original dataset. First, some abundance observations were not associated with a time of observation. We removed this data because popler can only accommodate population information associated with a time of observation. Second, a handful of abundance data points were clear typos (e.g. the letter "l" instead of a numeric value). We substituted these data points with a missing value (NULL in the database). We uploaded these pre-processed datasets in the popler database through a Graphic User Interface developed in Python using libraries panda and pyqt5.

Table S1: Taxonomic variables contained in the popler table on original taxonomic information.

Variable
sppcode
kingdom
subkingdom
infrakingdom
superdivision
division
subdivision
superphylum
phylum
subphylum
class
subclass
order
family
genus
species
common_name

Table S2: Metadata variables used to describe the datasets stored in popler.

Variable	Description
proj_metadat_key	Unique ID
lter_project_key	ID of LTER site
lter_project_key	ID of LTER site
title	Title of study
samplingunits	Unit of measure (if any) referred to population data.
datatype	Data type: count, biomass, cover, density, and individual. These correspond to the tables in Fig. 1A.
structured_type_n	If individual data, this shows what type of structure is stored. A study can contain up to $n = 4$ types of structure.
structured_type_n_units	Unit of measure (if any) referred to structure data.
studystartyr	Start year of the study
studyendyr	End year of the study
duration_years	Duration of the study in years
samplefreq	Frequency of population census
studytype	Whether study is observational or experimental
community	Whether study includes single taxon (community = F) or multiple taxa (community = T)
spatial_replication_level_n_extent	Extent of spatial replication level number n. A dataset can have up to to 5 replication levels.
spatial_replication_level_n_extent_units	Unit of spatial extent of the n spatial replication level.
spatial_replication_level_n_label	Label of the spatial replication level (e.g. transect, plot, quadrat, ect.). The label of spatial replication level 1 is "site".
spatial_replication_level_n_number_of_unique_reps	The number of unique replicates for the nth level of spatial replication.
treatment_type_n	The type of treatment (e.g. resource manipulation). A study can contain up to n = 3 treatments.
control_group	If study is experimental, this shows the field(s) that identify the control replicate.
derived	Is population size data raw, or is it derived (e.g. it is aggregated)?
authors	Author(s) of the original dataset
authors_contact	Email address(es) of the author(s) associated with the original dataset.
metalink	url of the original dataset
knbid	Knowledge Network for Biocomplexity identifier.

Table S3: LTER identification acronyms and their meaning as used in the `popler` database. *[These are not 28: I need to update list by final draft]*

Variable	LTER name
SBC	Santa Barbara Coastal LTER
SEV	Sevilleta LTER
SGS	Shortgrass Steppe
VCR	Virginia Coastal Reserve LTER
AND	Andrew Forest LTER
NWT	Niwot Ridge LTER
BNZ	Bonanaza Creek LTER
CDR	Cedar Creek Ecosystem Science Reserve
GCE	Georgia Coastal Ecosystems LTER
ARC	Arctic LTER
CAP	Central Arizon - Phoneix LTER
FCE	Florida Coastal Everglades LTER
HFR	Harvard Forest LTER
KBS	Kellogg Biological Station LTER
CWT	Coweeta LTER
HBR	Hubbard Brook LTER
MCM	McMurdo Dry Valleys LTER
JRN	Jornada Basin LTER
CCE	California Current Ecosystem LTER
KNZ	Konza Prairie LTER