



The AmeriFlux data activity and data system

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The AmeriFlux data activity and data system: an evolving collection of data management techniques, tools, products and services

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Received: 30 January 2013 – Accepted: 31 January 2013 – Published: 21 February 2013

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Published by Copernicus Publications on behalf of the European Geosciences Union.

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Abstract

The Carbon Dioxide Information Analysis Center (CDIAC) at Oak Ridge National Laboratory (ORNL), USA has provided scientific data management support for the US Department of Energy and international climate change science since 1982. Among the many data archived and available from CDIAC are collections from long-term measurement projects. One current example is the AmeriFlux measurement network. AmeriFlux provides continuous measurements from forests, grasslands, wetlands, and croplands in North, Central, and South America and offers important insight about carbon cycling in terrestrial ecosystems. To successfully manage AmeriFlux data and support climate change research, CDIAC has designed flexible data systems using proven technologies and standards blended with new, evolving technologies and standards. The AmeriFlux data system, comprised primarily of a relational database, a PHP based data interface and a FTP server, offers a broad suite of AmeriFlux data. The data interface allows users to query the AmeriFlux collection in a variety of ways and then subset, visualize and download the data. From the perspective of data stewardship, on the other hand, this system is designed for CDIAC to easily control database content, automate data movement, track data provenance, manage metadata content, and handle frequent additions and corrections. CDIAC and researchers in the flux community developed data submission guidelines to enhance the AmeriFlux data collection, enable automated data processing, and promote standardization across regional networks. Both continuous flux and meteorological data and irregular biological data collected at AmeriFlux sites are carefully scrutinized by CDIAC using established quality-control algorithms before the data are ingested into the AmeriFlux data system. Other tasks at CDIAC include reformatting and standardizing the diverse and heterogeneous datasets received from individual sites into a uniform and consistent network database, generating high-level derived products to meet the current demands from a broad user group, and developing new products in anticipation of future needs. In this paper, we share our approaches to meet the challenges of standardizing, archiving and delivering quality,

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well-documented AmeriFlux data worldwide to benefit others with similar challenges of handling diverse climate change data, to further heighten awareness and use of an outstanding ecological data resource, and to highlight expanded software engineering applications being used for climate change measurement data.

1 Introduction and background

1.1 Brief overview of the AmeriFlux network

The AmeriFlux network is a collection of more than 150 past and present flux towers (Fig. 1) located mostly in the United States, but with limited sites in Canada, Central America, and South America, making continuous measurements of water vapor, carbon dioxide (CO₂), energy fluxes, and related environmental variables using eddy covariance techniques (Baldocchi, 2003). The network covers a large variety of ecosystem types including forests, grasslands, croplands, shrublands, wetlands, savannas, and others (e.g., urban) (Fig. 2). The Carbon Dioxide Information Analysis Center (CDIAC) at Oak Ridge National Laboratory (ORNL), USA serves as the AmeriFlux permanent data archive and focal point for dissemination of AmeriFlux data (<http://public.ornl.gov/ameriflux>). As scientists and the public try to better understand climate change, AmeriFlux data have detailed how diverse ecosystems respond to changes in their physical environment and how ecosystems, in turn, affect their environments. AmeriFlux data have improved understanding of changes in net carbon uptake with interannual variation in climate and the influence of disturbance on carbon storage and fluxes. Models are fundamental to understanding and predicting biogeochemical cycles and future climates. AmeriFlux data are proving invaluable in improving and calibrating models used in climate science (e.g., Randerson et al., 2009; Schwalm et al., 2010; Williams et al., 2012).

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1.2 Challenges, design criteria, and requirements

Numerous challenges face CDIAC in organizing, managing, and distributing the AmeriFlux data collection from network operation challenges to software engineering challenges. The breadth and diversity of measurements made at individual sites, the variability of data processing performed by individual AmeriFlux sites, the absence of standardized nomenclature and metadata standards for handling ecological and micrometeorological data, the need to track data provenance, and the difficulties of securing detailed metadata necessary to fully understand and evaluate site measurements serve as examples of challenges addressed by CDIAC in constructing the network-wide AmeriFlux data system.

AmeriFlux sites are funded by multiple sources, typically US federal agencies. Recommendations are made by an AmeriFlux Scientific Steering Committee (SSC) regarding standard operating procedures, but there are no mandatory measurement and instrumentation protocols. Science objectives and corresponding measurement strategies are often site specific resulting in great variance, and richness, in the measurements made across the collective AmeriFlux network. Other regional flux networks exist worldwide, and coordination with these networks is important to optimize the utility of the AmeriFlux data collection and to better serve the larger climate change scientific community.

The AmeriFlux SSC and CDIAC offer guidance on data submission requirements to site investigator teams for continuous measurements and infrequent, complementary biological measurements. Raw data captured by the site data loggers for continuous measurements are maintained by the site teams and are not submitted to CDIAC. Site investigators process high frequency samples (usually at 10 Hz or higher) to produce half-hourly or hourly estimates of measured variables. Independent biological and ecological measurements (e.g., soil carbon content, foliage nitrogen concentration, tree allometry) are important for interpreting and validating the continuous AmeriFlux eddy covariance measurements and for parameterizing models. These companion biological

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measurements pose a challenge in assembling a consistent, network-wide resource due to the range of measurement methodologies and frequencies, differences in spatial representativeness, and the detailed metadata needed to fully characterize the measurement.

5 The breadth and diversity of measurements and data processing at individual sites, along with site differences in resources and staff dedicated to data handling, makes uniform data submission difficult. Data quality and consistency vary across AmeriFlux sites and measurement groups. As a result, CDIAC is tasked with assembling a network-wide database based on varying submissions from individual sites.

10 Adequate description of AmeriFlux measurements is crucial to proper use and understanding of reported AmeriFlux data. Metadata must be coupled with the primary environmental measurements to understand the reported data and expand use. Many micrometeorological and ecological terms commonly reported by AmeriFlux investigators are not covered by ongoing attempts to unify and standardize environmental data and metadata collections. For example, soil temperature and moisture measurements at various depths below the surface, which are commonly reported by AmeriFlux sites and fundamental to the AmeriFlux data collection, are not covered in the present NetCDF Climate and Forecast (CF) metadata convention.

20 AmeriFlux data records can be updated frequently as improvements (e.g., new screening algorithm) and adjustments (e.g., apply a correction to a degrading PAR sensor) are made to site data records. These changes must be documented making data provenance an essential ingredient of the AmeriFlux data system.

25 No single commercial software package or software engineering technique satisfies all the requirements for the AmeriFlux data system although the prototype Microsoft (MS[®]) DataCube was considered. Below we provide an overview of a comprehensive, data management approach used by CDIAC to handle Earth system data from the AmeriFlux network. We detail the software engineering techniques and tools used in the AmeriFlux data effort in the hopes other scientific data efforts will benefit from our experiences and these tools.

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2 Data management methods and approaches

2.1 Data submission, quality control and standardization

As mentioned previously, CDIAC is charged with assembling a network-wide AmeriFlux database from data submissions by individual site teams. CDIAC developed data submission guidelines (<http://public.ornl.gov/ameriflux/data-guidelines.shtml>) for the continuous half-hourly or hourly estimates of flux and meteorological variables to improve efforts in automating data processing and to invoke standardization of reported variables, units, and conventions (e.g., terrestrial carbon source and sink sign conventions).

To encourage data submissions, CDIAC accepts data in the manner most convenient for the submitting site team. Hourly or half-hourly summaries are received and obtained in numerous ways including mirroring scripts (wget and cron jobs), commercial transfer packages (e.g., Dropbox), dedicated areas on secure File Transfer Protocol (FTP) servers, or as e-mail attachments.

Due to differences in measurement strategies, data processing rigor, and data quality, CDIAC invests considerable effort to first evaluate submissions by individual site teams and then reformat, convert, or derive variables according to the prescribed submission guidelines (Table 1). A key initial task is to fully understand the content and context of the submitted data before producing a consistent network resource and this elementary step requires micrometeorological expertise. Fundamental groundwork is laid during this initial evaluation towards standardizing variable names, units, and reporting intervals and towards capturing and enhancing metadata.

Given the importance and diversity of AmeriFlux data and recent scrutiny towards climate change data and model results, it is imperative that scientific data archives address and document data quality. Permanent scientific data archives, like CDIAC, cannot accept data at face value without evaluating data quality or trusting quality assessments by data providers or outside assessment groups. CDIAC scrutinizes the continuous meteorological and flux data submitted by AmeriFlux investigators for quality

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changes if data providers fail to follow the submission guidelines in their original submissions. Typical examples are unit conversions (from g dry biomass m^{-2} to $g C m^{-2}$), adjustments to conform to prescribed definitions (from double-sided and all-sided leaf area indices to single-sided), and data code translations (replacing the scientific and common names of tree species by their standard codes defined by the United States Department of Agriculture, Natural Resources Conservation Service).

2.2 Products

CDIAC offers four different product levels for the continuous AmeriFlux meteorological and flux measurements. These products differ in origin, content, and level of data processing. The four product levels are:

- Level 1 – processed data provided by the site investigators. Level 1 data files originally provided by the site measurement teams are evaluated and corrected by CDIAC as described in Sect. 2.1 and further processed by CDIAC to produce Level 2 data products. The Level 1 data files are posted in their original form on the publically-available CDIAC anonymous FTP server (<ftp://cdiac.ornl.gov/pub/ameriflux/data/>) and include regular and continuous half-hourly or hourly measurements of flux and meteorological variables and irregular measurements of biological variables in the BADM template or site specific format.
- Level 2 – data checked and formatted by CDIAC. Data received from individual sites are reviewed, quality-controlled, reformatted, and incorporated into a network-wide AmeriFlux database. The review or evaluation process includes checks for consistent units, naming conventions, reporting intervals and others (see Sect. 2.1) and reformatting is often necessary to maintain consistency within the larger network-wide database. Level 2 data include both regular and continuous measurements of flux and meteorological variable and irregular measurements of biological variables. Considering the breadth and diversity of measurements at AmeriFlux sites, it is necessary for CDIAC to generate Level 2

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individual measurement variables over time or plots of two correlated variables. The old adage – “One Picture is Worth a Thousand Words” is very true when evaluating scientific data. SAS[®] graphics capabilities complement the routine CDIAC quality checks summarized in Table 2 and often highlight obvious quality issues in the incoming data (Fig. 5). Another nice feature of the SAS[®]/IntrNet product is the ability to produce automated metadata reports in HTML format documenting data provenance including variable mappings, calculations, and unit conversions, etc.

CDIAC archives and distributes AmeriFlux data across two systems: (1) a PHP-based web-interface that draws on a MySQL relational database; and (2) an anonymous FTP server. The two systems are independent but connected by links in the PHP web-interface pointing to the FTP server.

Once CDIAC data quality checks are complete, the AmeriFlux Level 2 data in the form of a SAS[®] database are ingested directly into an AmeriFlux MySQL relational database using a PHP script. PHP is an advanced web-programming language that enables programmers to construct complicated web sites without compromising server-site processing abilities, an important consideration for the AmeriFlux system given the anticipated multi terabyte-level data volumes. MySQL at the same time is a powerful, robust, and flexible open-source product capable of handling large volumes of complex Earth system data. MySQL design architecture enables environmental programmers to partition large data volumes and thus increase query performance. For AmeriFlux data, it was logical to implement site-based partitioning since the data collection is built on data streams provided by individual site teams. Site investigators and identifiers serve as common threads linking MySQL tables comprising the AmeriFlux relational database (Fig. 6). Another important decision was made early in the AmeriFlux data architecture design to handle all data additions and corrections via a PHP-developed, web-based editing interface. This strategy allows CDIAC to control the content of the production and archive databases, automate data movement, track data provenance (i.e., track changes, assign version numbers, etc.), and manage metadata content and standardization. The strategy also removed the need for

client-side software distributions. Presently, over 500 million observations reside in the production-side AmeriFlux MySQL database available to the public.

The primary tool to deliver AmeriFlux data is a web-based interface referred to as the AmeriFlux Site and Data Exploration System (<http://ameriflux.ornl.gov>). The PHP interface allows users to query the AmeriFlux MySQL database in a variety of ways. Anticipated popular data and metadata search criteria were identified by CDIAC staff and incorporated into the interface to assist users to navigate through the AmeriFlux database. Examples of search criterion are product levels (see Sect. 2.2), dates of available data, ecosystem types, site operating status (i.e., active or inactive), site coordinates, and instruments. New scientific-based search criteria are being added (e.g., distinction of measurements between nighttime and daytime, growing and dormant seasons) based on emerging needs from climate change researchers. Once users have identified data of interest, the interface permits users to further subset, download, or visualize their selections. The same interface can be used to obtain fundamental site information for all registered AmeriFlux sites. Independent web pages are dedicated to every single site and users can browse a broad set of metadata for the site of interest. These metadata include, for example, site identification, coordinates, names of principal investigator(s), site instruments and publications, descriptions of site climate, vegetation, soil, terrain and land use history, and many others. Interactive tables list all measurements reported by a site including variable names, definitions, units, and sign conventions. Visualization capabilities are also available at this web-interface. Data can be downloaded directly from the AmeriFlux MySQL database through this web-interface or from the links pointing to the CDIAC FTP server.

As described in Sect. 2.2, CDIAC generates a set of Level 2 standardized ASCII data files for flux and meteorological variables. These Level 2 files are posted on the CDIAC anonymous FTP server (<ftp://cdiac.ornl.gov/ameriflux/data/Level2>) after being created using SAS[®] codes. These files are posted in separate site folders identified by the site name or a unique site ID (e.g., US-UMB) assigned to all flux sites worldwide. To satisfy users interested in data from multiple AmeriFlux sites rather than an

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individual site, “Unix tar balls” are created and posted on the same CDIAC anonymous FTP server. New “tar balls” are created whenever new AmeriFlux standardized files are posted to the FTP server using a Perl script which executes based on new files names and creation dates. The “tar ball” file name conveys the creation date to promote easy mirroring and citation by users. These standardized files serve another critical function. They enable the AmeriFlux regional network to participate in a virtual global flux network (FLUXNET) and its cross-continent synthesis studies. To further aid modeling and synthesis activities, identical NetCDF files are produced from the Level 2 standardized files using a Perl script to reformat the standardized files into the file format required by the NetCDF Compiler. All header information provided in the standardized ASCII files is written as global attributes into the corresponding NetCDF files. These NetCDF files are posted to the CDIAC server and included in the above-mentioned “tar balls”.

Also available at this FTP server are the higher level data products (i.e., Level 3 and 4 data) and biological data. After scrutinizing the biological data (see Sect. 2.1), individual BADM files are integrated into a single MS Excel[®] file with multiple spreadsheets dedicated for different categories of biological measurements, including lead area index (LAI), soil respiration, stand properties, biomass production, vegetation C and N content, soil properties, and phenology. This integrated file, also referred to as Level 2 biological data, is entered into the AmeriFlux MySQL database by CDIAC staff through the PHP editing interface and also posted to the AmeriFlux FTP server. The complete AmeriFlux data life cycle, from site collection to distribution by CDIAC, is shown in Fig. 7.

Two additional expanding systems are used to further promote and broadcast CDIAC’s AmeriFlux data products and services. First, CDIAC deploys a Mercury instance. Mercury is a web-based, distributed metadata management, data discovery, and data access system (<http://mercury.ornl.gov>) implemented using Internet standards, including XML, and supports international metadata standards including FGDC, Dublin-Core, EML, and ISO-19115. CDIAC produces metadata summaries for AmeriFlux data products for inclusion in the CDIAC Mercury instance (<http://mercury.ornl>).

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gov/cdiac/) using a customized on-line metadata editor (OME). OME produces XML files for ingest, cataloging, and indexing by the CDIAC Mercury instance and other disparate climate-change related Mercury instances. Secondly, CDIAC AmeriFlux data products are being published into the Earth System Grid Federation (ESGF). ESGF is a data distribution portal used primarily to distribute large-scale, modeling results (Williams et al., 2009). ESGF integrates supercomputers with petabyte-scale data and analysis servers located at national labs and research centers to create a powerful environment for next generation climate research. ESGF served as the focal point for disseminating results from the Intergovernmental Panel on Climate Change (IPCC) Fourth Assessment Report (AR4) and will serve in a similar capacity for the IPCC Fifth Assessment Report (AR5). ESGF has historically focused on model output, but is now including observational data important for model testing and validation, including AmeriFlux data provided by CDIAC (<http://esg2-gw.ccs.ornl.gov>).

3 Conclusions

Like most scientific computing endeavors, there is no ready, commercial product that satisfies the full suite of data analysis, data management, metadata management, and data delivery requirements for the AmeriFlux data activity. The breadth, complexity, and variability of data and metadata are too great to be handled by a single tool or product. Instead, CDIAC has deployed a variety of data management tools, software, and software engineering techniques to support the AmeriFlux data activity. Where needed, tools and applications have been adapted and modified to specific requirements driven by the data needs of the international climate change research community. Scientific data management approaches must be flexible, portable, and expandable in order to accommodate future users, increased data volumes, and new data products. It is virtually impossible to predict all future applications of scientific data making it imperative that data system designs be flexible for unanticipated growth and, more importantly, that detailed metadata be captured to promote unexpected use and application.

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Immediate needs for the AmeriFlux data system demonstrate the need for flexibility. There is a need for synchronization of regional flux databases including common variable nomenclatures and units, common data products and metadata, uniform data processing, and node access to a “global” flux database. As publication tools for observational databases are developed within the ESGF, there will be a need to automate the ingest of AmeriFlux data to ESGF and further to launch new model simulations as revised and updated AmeriFlux data become available. Demand from the scientific community and general public has grown for inclusion of uncertainty estimates or error bounds on flux and meteorological data. CDIAC is now undertaking an effort to provide uncertainty estimates in the AmeriFlux data system and developing other products such as derivation of phenology stages from the existing measurements at AmeriFlux sites.

Acknowledgements. This research and CDIAC were supported by the US Department of Energy, Office of Science, Biological and Environmental Research (BER), and conducted at Oak Ridge National Laboratory (ORNL), managed by UT-Battelle, LLC, for the US Department of Energy under contract DE-AC05-00OR22725.

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Table 1. Initial checks, evaluations, and clarifications performed by CDIAC on incoming AmeriFlux meteorological and flux data. These checks are necessary to determine the content and quality of the submitted data, as well as to identify corrections and derivations that must be made in subsequent processing.

Categories used to evaluate incoming AmeriFlux data	Considerations and examples
Time representation	Are the data time-stamped using local time or Universal Standard Time (UST)? Are values reported at the beginning or ending of a sampling period?
Variable nomenclature, definition, and symbolic convention	What measured and derived variables are provided and how are they named or represented symbolically? For example, water vapor flux vs. evapotranspiration or different acronyms (PAR vs. PPF) for the same measurement of photosynthetically active radiation. How is each variable defined? For example, is soil heat flux defined as heat flux through the soil heat plate or as the sum of the heat flux through the soil heat plate and the heat stored in the soil layer above the plate?
Unit	What unit is used for each reported variable and is it consistent with the prescribed data submission guidelines? For example, reporting CO ₂ concentration in $\mu\text{mol mol}^{-1}$ vs. mg m^{-3} .
Sign convention	What sign conventions are used by the reporting team? For example, carbon uptake is often reported as negative values for downward CO ₂ fluxes but as positive values for upward releases to the atmosphere from photosynthetic production.
Multiple and redundant measurements	Are multiple and redundant measurements reported and, if so, how are they represented? For example, are they reported as independent measurements or an average from multiple sensors?
Measurement height/depth	Is each measurement properly associated with a measurement height or depth? Are values reported at a single level or reflecting an integral measurement of multiple levels? For example, soil temperature measured at 10 cm vs. within a vertical column (0–30 cm).
Data handling and processing	What adjustments have been applied to the reported variables? Were the data filtered, screened, or gap-filled? Were corrections applied to the flux terms and, if so, which ones (e.g., planar vs. two-dimensional coordinate rotation)?
Metadata	Are the submitted data accompanied by proper metadata? Different measurement teams report different levels of details in their metadata, from simple file headers (symbolic variable names and units only) to comprehensive documentation including measurement techniques, variable definitions, sign conventions, etc.
Basic data quality assessment	Are the data submitted of “publication” quality or just one step after being retrieved from the data-logger?

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Table 2. Quality evaluations and checks performed by CDIAC on incoming meteorological and flux data submissions.

Quality evaluations/checks	Detail and action
Missing or repeated entry	Determine if the total number of yearly data records matches the expected total (e.g., 17 520 half-hourly records for a non-leap year), if the time increment between consecutive entries matches the sampling intervals (30 or 60 min); and if data entries are in chronological order
Time-stamp	Check for consistency between time-stamp entries, for example, between a set of month, day, hour, minute and Julian day entries
Threshold	Conservative thresholds are determined for each variable and site (e.g., the likely maximum air temperature at an Alaskan site), and out-of-bound values are reset to a prescribed missing value (e.g., -9999)
Nighttime radiation	Determine the daily nighttime period using a sunrise and sunset calculator and the percentage of nighttime radiation values beyond a tolerance level; these invalid values (for shortwave and photosynthetically active radiation) are reset to zero
Biological and meteorological inter-relationship	Some variables or redundant measurements should be inherently correlated, for example, photosynthetically active radiation and global radiation, air temperature and soil temperature, etc. Poor correlations typically indicate problems and are investigated on a case-by-case basis
Spike detection	Generally speaking, a data value is considered a “spike” if the value deviates from the mean by ± 3 standard deviations. For variables with little expected variation (e.g., pressure), we check for spikes over the entire time series. For variables showing distinct seasonal and diurnal patterns (e.g., air temperature), we check for spikes against the diurnal means within a moving time window (e.g., 20 days)
Stationarity	Check if time series lack reasonable variation during a day or over a short period (10–20 days)
Diurnal and seasonal cycles	Check the monthly mean diurnal cycles and seasonal cycles where these cycles are known and expected; diurnal cycle for a single day is checked by evaluating the correlation and consistency between this day and the mean diurnal cycles in the current and neighboring months
Discontinuity and inter-annual variation	Detect the discontinuities and trends in time series across multiple years. For example, a declining trend in radiation measurement over years may indicate an instrument calibration drift

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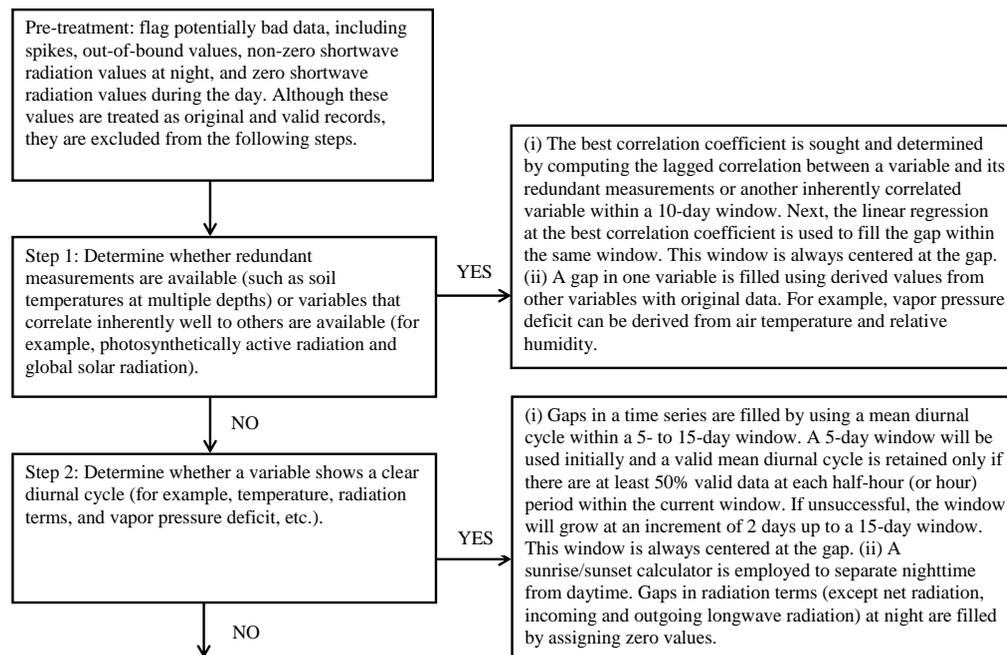
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Table 3. Flow diagram for the methodology used by CDIAC to gap-fill meteorological records for the AmeriFlux network.

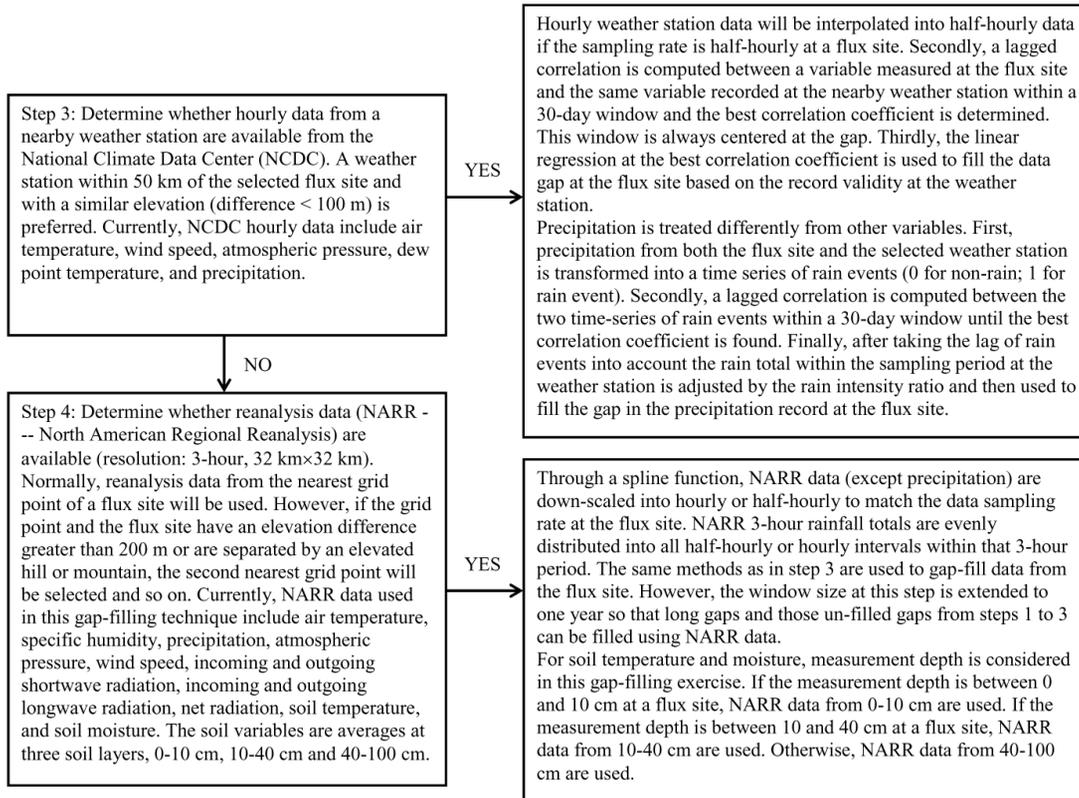


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Table 3. Continued.



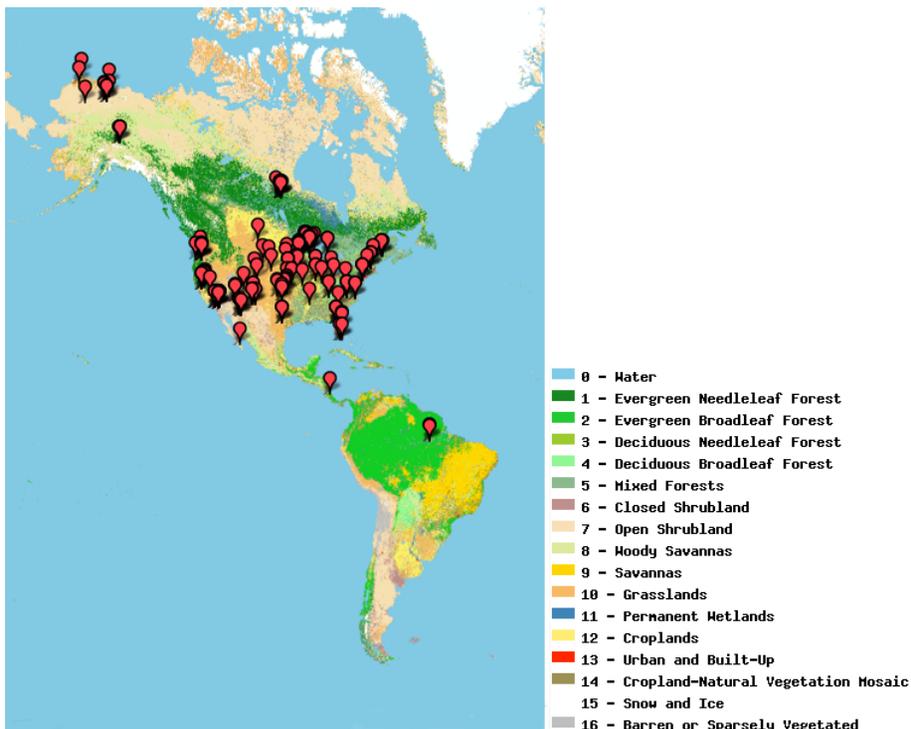


Fig. 1. Geographic distribution of registered flux sites in the AmeriFlux network as of January 2013 superimposed on a map depicting ecosystem representations from the International Geosphere-Biosphere Programme (IGBP).

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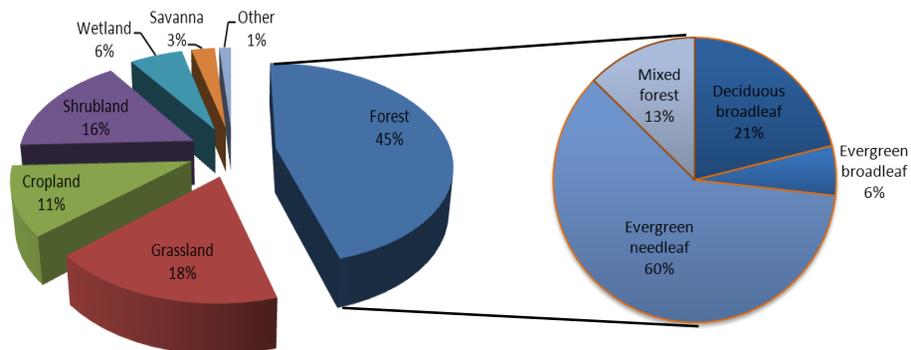


Fig. 2. Ecosystem representation, according to IGBP ecosystem classifications, of the AmeriFlux network based on registered sites as of January 2013.

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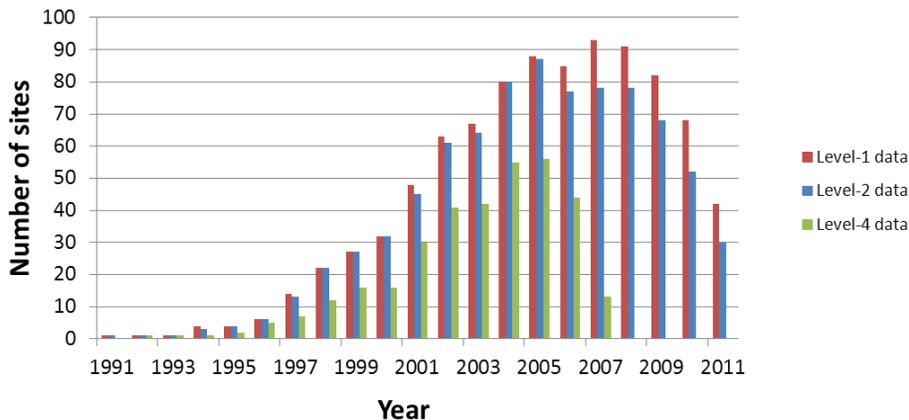


Fig. 3. Number of AmeriFlux sites with data for each year from 1991 to 2011 based on the CDIAC AmeriFlux data collection in January 2013.

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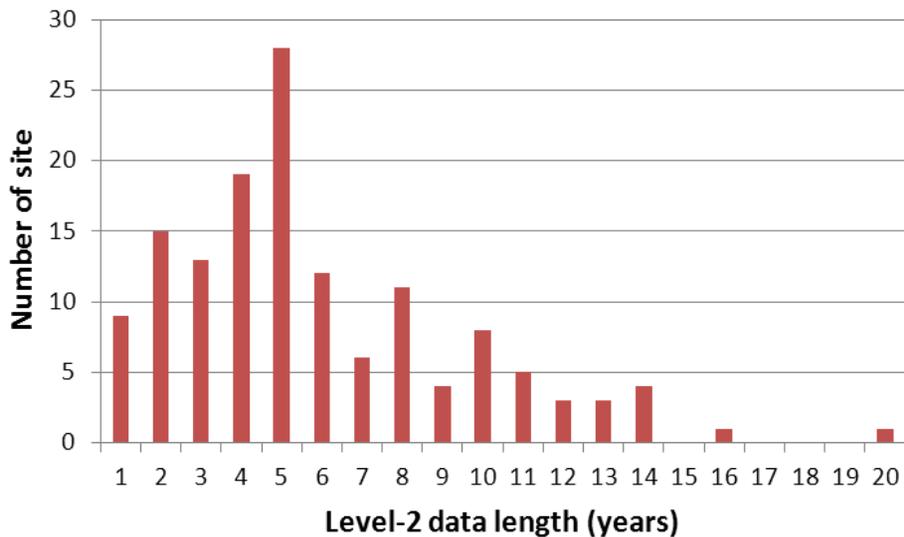


Fig. 4. Distribution of data record lengths in years for the 142 AmeriFlux sites with available Level 2 data products based on the CDIAC AmeriFlux data collection in January 2013.

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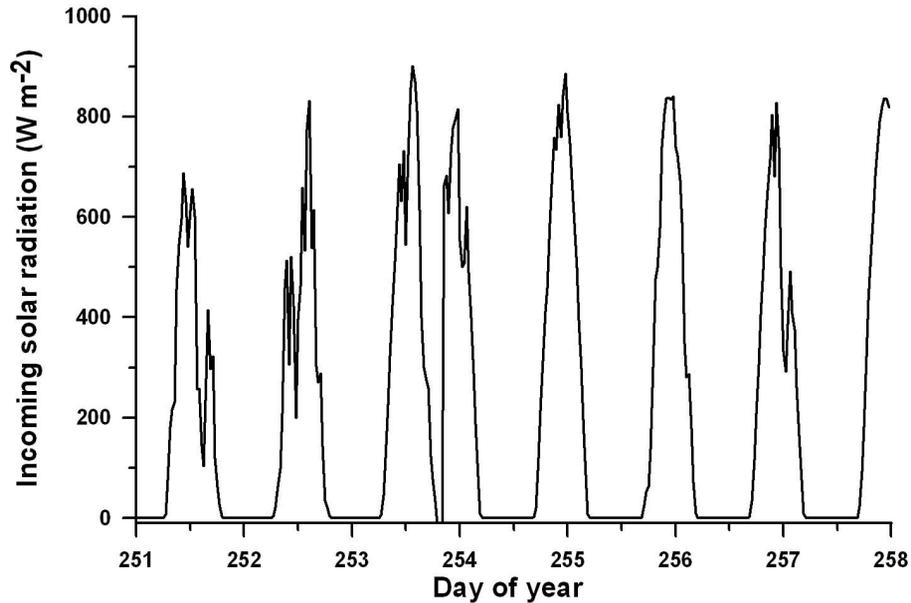


Fig. 5. CDIAC uses graphics and visualization tools to review time series for all measured AmeriFlux variables, assess data quality, and identify possible errors. This plot shows an erroneous time shift beginning on day 254 for incoming solar radiation.

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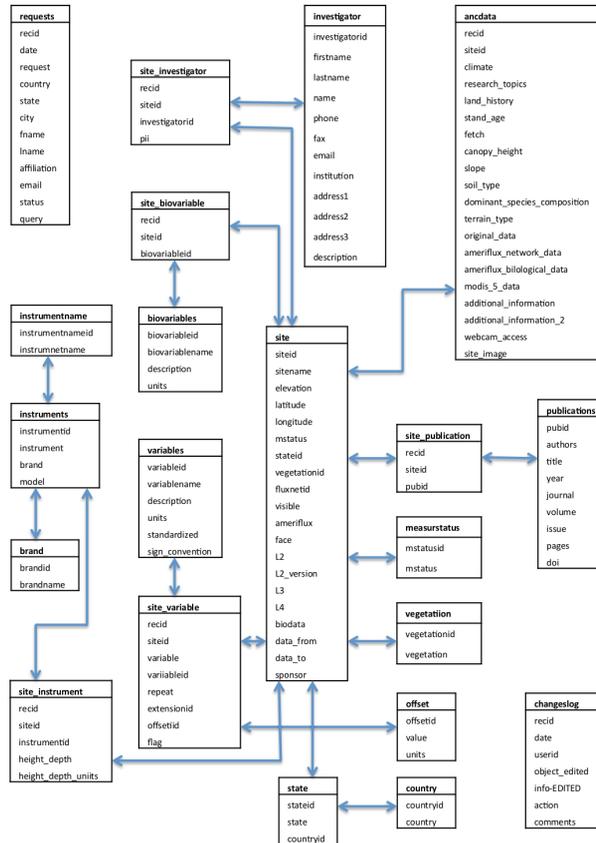


Fig. 6. Diagram identifying the tables comprising the CDIAC AmeriFlux MySQL relational database. Tables connected by arrows share two identical variables, the site identifier and site investigator, to enable queries across multiple tables. Tables not connected by arrows are stand-alone tables within the database. Table names are shown at the top of each table box in bold letters. Column names within each table are listed below the table names.

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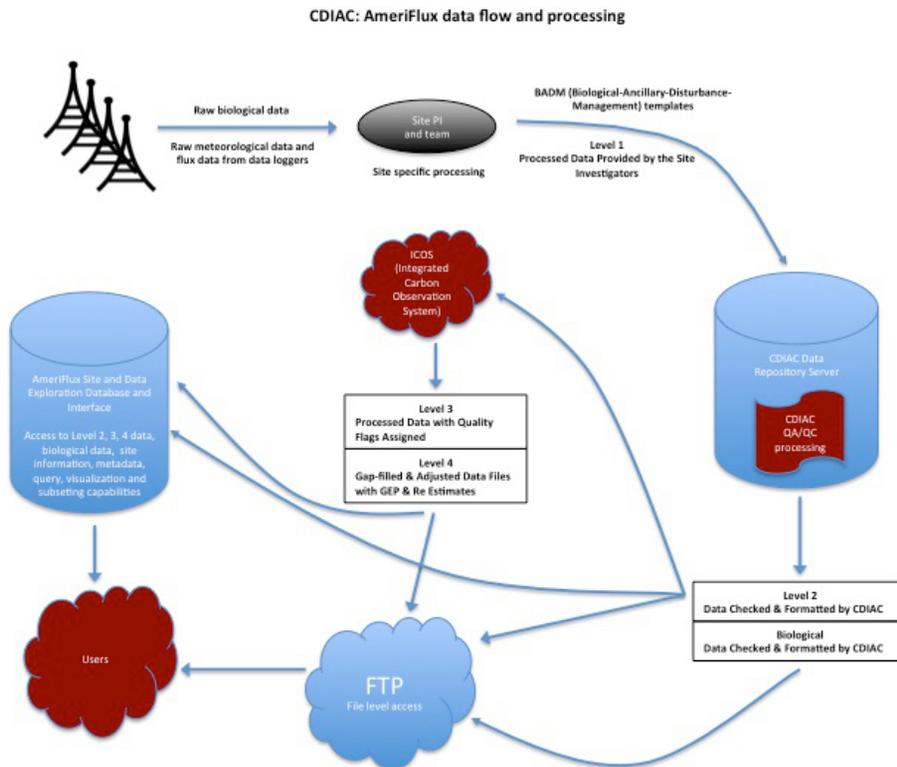


Fig. 7. The AmeriFlux data life cycle. The life cycle moves from site collection (upper left) to processing by the site teams (top center) to CDIAC processing and data product generation (right side) to Integrated Carbon Observing System processing and product generation to dissemination by CDIAC.

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