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SoDaH: the SOils DAta Harmonization database, an open-source synthesis of soil data from research networks, version 1.0.

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Abstract. Data collected from research networks present opportunities to test theories and develop models about factors responsible for the long-term persistence and vulnerability of soil organic matter (SOM). Synthesizing datasets collected by different research networks presents opportunities to expand the ecological gradients and scientific breadth of information available for inquiry. Synthesizing these data, are challenging, especially considering the legacy of soils data that has already been collected and an expansion of new network science initiatives. To facilitate this effort, here we present the SOils DAta Harmonization database (SoDaH; https://lter.github.io/som-website, last accessed 15 July 2020), a flexible database designed to harmonize diverse SOM datasets from multiple research networks. SoDaH is built on several network science efforts in the United States, but the tools built for SoDaH aim to provide an open-access resource to facilitate and automate further harmonization and synthesis of soil carbon data. Moreover, SoDaH allows for individual locations to contribute results from experimental manipulations, repeated measurements from long-term studies, and local- to regional-scale gradients across ecosystems or landscapes. Finally, we also provide data visualization and analysis tools that can be used to query and analyze the aggregated database. The SoDaH v1.0 dataset is archived and available at https://doi.org/10.6073/pasta/9733f6b6d2ffd12bf126dc36a763e0b4 (Wieder et al., 2020).

1 Introduction

Soil organic matter (SOM) contains two- to three-times the amount of carbon (C) as the atmosphere and terrestrial vegetation combined, yet adequately describing SOM dynamics in numerical models remains a challenge (Jackson et al. 2017). Recent biogeochemical research has attempted to understand how climate, biota, soil chemistry, and mineralogy interact to determine SOM stabilization and persistence (Schmidt et al. 2011; Lehmann & Kleber 2015). Emerging theories also highlight how interactions among these factors affect the production and apparent stabilization of microbial residues (Grandy & Neff 2008;

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Cotrufo et al. 2013; Kallenbach et al. 2016). Notably, these new studies emphasize the importance of soil mineralogy and physical structure in limiting microbial access to otherwise decomposable substrates (Dungait et al. 2012; Miltner et al. 2012; Schimel and Schaeffer 2012; Sulman et al. 2014).

Datasets that span environmental and edaphic gradients are critical for constraining soil C estimates and developing and testing theoretical and numerical models that are based on these ideas (Wieder and Allison et al. 2015; Luo et al 2016; Harden et al. 2018; Sulman et al. 2018; Malhotra et al. 2019). Data synthesized across scientific networks, notably those with long-term observations and manipulations, are especially useful for establishing general patterns across broad environmental gradients. These insights, and the raw data are valuable for model development. For example, efforts to synthesize and archive results from the Long-Term Intersite Decomposition Experiment Team (LIDET; Gholz et al. 2000; Parton & Silver et al. 2007; Adair et al. 2008; Harmon 2013) provide a valuable benchmark for parameterizing and evaluating models with litter decomposition data (Bonan et al. 2013; Wieder and Grandy et al. 2015; Kyker-Snowman et al. 2019). Elsewhere, Zhang et al. (2020) used data from three research networks in Europe, China, and Australia to parameterize and evaluate two soil carbon models. Providing similar data products in public databases is critical to advancing understanding soil biogeochemistry.

Coordinated research activities and the expansion of research network infrastructure are broadening the scope and breadth of information measured across sites in ways that can advance SOM science (Hinckley et al. 2016; Baatz et al. 2018; Richter et al. 2018; Weintraub et al. 2019, Lajtha et al. 2018). With a 40-year investment in continuous or multi-year measurements and a rich legacy of manipulative experiments, the Long-Term Ecological Research (LTER) Network provides a publicly available data archive through the Environmental Data Initiative (EDI; https://portal.edirepository.org/nis/home.jsp). The LTER network has an advantage of hosting diverse research experiments, but because each site in the network has different research foci data are not collected or reported in a consistent manner (Billings et al. 2020, but see Zak et al. 1994; Frank et al. 2012). By contrast, new investments in networks like the National Ecological Observatory Network (NEON) provide a top-down, standardized framework for data collection across sites. Synthesizing data from across LTER, NEON and other research networks present unique opportunities to deepen our general understanding of soil biogeochemistry.

Here, we present a flexible database designed to harmonize diverse SOM datasets from across research networks. We aim to provide an open-access resource to facilitate and automate further harmonization and synthesis of soil C data. This data resource can expand to accommodate legacy datasets as they are identified and incorporate new data products as they become available. This data infrastructure is critical to advance understanding in SOM dynamics at a time when the theoretical foundations and numerical representations of soil biogeochemical processes are rapidly evolving.

2 The SoDaH database

Our team created the SOils DAta Harmonization (SoDaH) database to bring together soil C data from diverse research networks into a harmonized dataset that can be used for synthesis activities and model development. The research network

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sources for SoDaH span different biomes and climates, encompass multiple ecosystem types, and have collected data across a range of spatial, temporal, and depth gradients. The rich data sets assembled in SoDaH consist of observations from monitoring efforts and long-term ecological experiments. The SoDaH database also incorporates related environmental covariate data pertaining to climate, vegetation, soil chemistry, and soil physical properties. The data are harmonized and aggregated using open-source code that enables a scripted, repeatable approach for soil data synthesis. Finally, to accompany SoDaH, we provide data visualization and analysis tools that can be used to query and analyze the aggregated database.

2.1 Database Sources and Structure

Research networks provide a powerful observational platform for enhancing our understanding of ecosystems. For example, in the United States, three research networks funded by the National Science Foundation collect soils data that deepen understanding and improve the representation of soil biogeochemical processes in models. These include the LTER network (https://lternet.edu/), Critical Zone Observatories and their successor sites (CZO; http://criticalzone.org/national/), and the National Ecological Observatory Network (NEON; https://www.neonscience.org/, NEON 2020). Other coordinated research activities that further expand data availability include community efforts like the Nutrient Network (NutNet; https://nutnet.org/) and Detritus Input and Removal Treatments (DIRT; https://dirtnet.wordpress.com/). We compiled soils data from these five research networks into the SoDaH database, version 1.0.

The unique perspectives and historical legacies of each network synergistically offer insights into understanding many aspects of SOM dynamics. For example, data from LTER, DIRT and NutNet sites are generally long-term datasets that focus on surface soil (< 30 cm) properties across gradients and response to experimental manipulations. Data from CZO sites tend to contribute information on soil geochemical properties and expand focus to include deeper (> 30 cm) soil horizons. Finally, NEON employs standardized data collection procedures that span continental-scale ecoclimatic gradients (Fig 1).

The SoDaH dataset focuses on soil organic carbon (SOC) concentration (% C), estimated SOC stocks (g C m^{-2}), and associated covariates that may be useful in explaining variation in SOC stocks within and among sites. To avoid confounding the interpretation of SOC measurements collected by different approaches (e.g. Walkley-Black and mass loss on ignition), we focused on synthesizing SOC measurements from soil samples that were acidified if needed to remove inorganic carbonates, then analyzed for total C using elemental analyzer. Beyond SOC, covariates collected in SoDaH include abiotic factors (e.g., climate [mean annual temperature and precipitation], soil depth, bulk density, particle size distribution, and mineralogy), vegetation characteristics (including vegetation type and above and belowground root productivity, biomass, and chemistry), and additional soil chemical properties (total nitrogen, phosphorus, pH, etc.).

Recognizing that the cyber landscape of soil databases is expanding (Malhotra et al. 2019), we wanted to structure SoDaH in a manner consistent with existing databases, perhaps most notably the International Soil Carbon Network (ISCN; Nave et al. 2016, Harden et al. 2017), which similarly focuses on SOC concentrations and stocks in bulk soils. The ISCN uses a hierarchical data structure that links metadata information with fields for location, profile and soil layer data. We

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maintained the ISCN's basic structure in SoDaH (Fig. 2), as it provides a logical means to structure relationships between different measurements (i.e., variables). A similar approach was also used in the International Soil Radiocarbon Database (ISRaD; Lawrence et al. 2020), which primarily focuses on synthesis of additional information about C isotopes and soil fractions. Given this focus of ISRaD, the SoDaH database contains only sparse data on isotopes and SOM fractions. Since SoDaH and ISCN focus on SOC measurements and have a similar structure, we hope they may be used together in future studies.

The unique contribution from SoDaH, relative to other soil databases, is that SoDaH is built on several network science efforts in the United States, and presents a usable, extensible database for contributing and analyzing data. Moreover, SoDaH allows for individual locations to contribute results from experimental manipulations, repeated measurements from long-term studies, and local- to regional-scale gradients across ecosystems or landscapes. Thus, SoDaH allows for the harmonization of data spanning a greater range of spatial and temporal scales than other databases, and enables the incorporation of ecosystems responses to manipulations, which is not a possibility for other databases.

Given the focus on experimental manipulations, we requested additional categorical information on location and profile fields to clarify aspects of data collection and experimental design. This includes flags in the location field asking if datasets include measurements that are repeated over multiple time points, come from experimental manipulations, or represent gradient studies. We also asked dataset contributors to identify 'control' or unmanipulated sample identifiers when necessary. We accommodated various experimental designs and data hierarchies with fields to describe this information, such as whether plots are grouped into blocks or watersheds, and the organization of treatment levels, in the profile field of the database. For example, at one site, data may be collected from plots along an elevational transect; whereas, another dataset may include information from a nitrogen fertilization treatment that was conducted on experimental plots in a replicated block design. Maintaining these data hierarchies is important for database users to inform how best to aggregate data collected from diverse networks, individual study sites, and unique experimental designs.

2.2 Data Identification and Contributions

To begin populating the SoDaH database, we identified data contributors who were familiar with datasets available from individual study sites and research networks. Many of the datasets in SoDaH were already published in public repositories like EDI (the primary repository for LTER data), or available through the NEON data portal. Other datasets that we wanted to include in SoDaH, however, had not been published or were difficult to find or identify (mainly data from CZO sites and the DIRT network, but also some LTER data). Publishing these raw data remains an active priority for our working group. Data providers who were familiar with the diversity of datasets that are available at a study site or a network provided expertise to link soil C datasets with appropriate ancillary data.

The SoDaH database was constructed by data contributions from individual sites or research networks who provided flat (.csv) files to a shared directory on Google Drive. The dataset (or datasets) from each site, study, or network

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were placed in their own subdirectory along with a metadata template that was used to map variable names in the raw (Level 0, Fig. 3) data to the structure of SoDaH. The metadata template was developed to facilitate data harmonization in a scripted, repeatable manner that maintained the integrity of the raw datasets (https://lter.github.io/som-website/database.html). To simplify the workflow for data contributors, the metadata template only includes a single tab each for location and profile data; within these tabs, data contributors are able to add information on metadata, and layer fields (Fig. 2). This step of our data harmonization still requires manual effort from data providers, as they have to map the names of measured variables from raw data with the appropriate variable in SoDaH. Data contributors enter relevant metadata and site information that may not be included in the raw data sets. They provide additional information from controlled drop-down cells with information on units for each variable (e.g., %C, g C kg^{-1} soil, mg C kg^{-1} soil, etc.) or on methodologies used (e.g., soil P measured by Bray, Melich, etc.). In the harmonized dataset, we convert units to a standard output and include methodological information (section 2.3). This approach accommodates a broad suite of soil and related variables (e.g., climate, vegetation characteristics, ecosystem productivity, etc.). In the future, we aim to further reduce data provider input requirements, but only if the community converges on standardized variable names and units of measure (sensu Billings et al. in review). Ultimately, sophisticated metadata (e.g., ontologies of variables and units of measure) may facilitate automated harvesting of data from disparate networks and repositories.

The metadata template matches site-level information with the detailed measurements collected at each study site. Data on the profile tab corresponds to columns of variables that are reported in the raw data (e.g., soil C in each experimental plot). The metadata template assumes that data on the location tab represent site characteristics for a single site or location (e.g., Prospect Hill Warming experiment at Harvard Forest). The harmonization script copies each unique measurement from the profile tab into a column of data in the harmonized dataset. By contrast, data provided on the location tab (latitude, longitude, mean annual temperature, etc.) are broadcast to every row of the harmonized dataset. Data contributors, however, can move variables from the location to profile tabs when appropriate (e.g., moving site information on climate onto the profile tab for NutNet and NEON data).

The harmonization script can harmonize multiple datasets from the same study location. For example, a dataset may consist of multiple data files that each contain details about different aspects of the study (e.g., soil data in one file, aboveground productivity in another file); the harmonization script will harvest all variables identified in the metadata file from the suite of data files (as long as they are in the same Google directory as the metadata file). However, because SoDaH is a flat database, values from these different data files will be stacked, requiring additional aggregation steps to align data within sites.

2.3 Data Harmonization and Aggregation

We developed the *soilHarmonization* package in R (R Core Team 2020) to harmonize and aggregate the SoDaH database. The *soilHarmonization* package is publicly available (https://github.com/lter/soilHarmonization), and includes tools to read

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and harmonize user-provided raw data that are mapped to a metadata template with controlled vocabulary and standard units (Fig. 3). Users point to the Google Drive directory where Level-0 data are located (raw data and metadata template), and the *soilHarmonization* package generates a new flat file(s) in which the variable names and units, if relevant, are standardized in the output (Level-1 data). The harmonized dataset includes unique columns of data from those defined in the profile tab as well as columns of data with site-level information from the location tab. The package also includes a suite of QC tools that confirm proper data type (e.g., strings are not interspersed with numeric values) and that numeric data, once converted to appropriate units, fall within an expected range. A summary of inputs, outputs, homogenization steps, and a QC report are detailed in an accompanying document (.pdf) for each harmonized dataset. These Level-1 data products are stored in the same Google Drive directory as the Level-0 data with resulting output identified with a modified filename.

After generating Level-1 data from all Level-0 data, we combined harmonized data files into an aggregated dataset (.rds or .csv format; Fig. 3). This *dataHarvest* function (available on the LTER SOM GitHub page, https://github.com/lter/lterwg-som/tree/main/data-aggregation/, last accessed July 15, 2020) aligns columns of Level 1 data into a single, Level 2, dataset. The resulting SoDaH database (version 1.0) we describe here is a single, flat dataset that has columns corresponding to variables in the metadata template and rows for each measurement.

2.4 Data Visualization and Analysis

To facilitate user interaction with the SoDaH database, and to provide a simplified approach for data queries and analysis, we developed a web-based application using R Shiny (Chang et al. 2020). This SoDaH application is publicly accessible and hosted by the National Center for Ecological Analysis and Synthesis (NCEAS) at https://cosima.nceas.ucsb.edu/lter-som (last accessed July 15, 2020; source code: https://github.com/lter/lterwg-som-shiny). With the SoDaH application, users can interactively filter the SoDaH database by network, experiment type, and soil depth, and can selectively include or exclude experimental treatments or time-series data. User-defined data subsets may then be used to map soil C and other covariates or construct basic analysis plots (point, histogram, or boxplot) using both covariates (e.g., Fe concentration) and metadata (e.g., mean annual precipitation). Further, the user-specified data subset, or the entire SoDaH database, may be downloaded as a flat file (.csv) through the SodaH application. The SoDaH application also provides site-specific summary information and a key for the SoDaH database construct, including descriptions of database fields and their associated metadata.

For users seeking to move beyond the functionality provided by the SoDaH application, R scripts are provided through the LTER SOM GitHub repository (https://github.com/lter/lterwg-som/tree/main/data-projects, last accessed July 15, 2020) to facilitate and demonstrate scripting language to import, filter, summarize and map data from the SoDaH database. This repository is intended to facilitate use of the SoDaH database, and the scripts used to generate figures in this paper are available in the repository. We encourage database users to draw from these existing resources and contribute new scripts they develop for scientific analysis of data in SoDaH.

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Additional data aggregation steps may be required to fully realize strengths of the SoDaH database. These could include, identifying suitable approaches to aggregate, and aligning data within sites. The aggregation steps currently implemented in SoDaH may not be appropriate for particular research questions, especially those concerning spatial and temporal gradients. Therefore, users may need to align rows of data from the same profile or location, but were harvested from multiple data files, which results in data being stacked within the flat database. For example, a site may contribute data on soil chemical properties, soil physical properties, microbial stoichiometry and biomass, litterfall chemistry, and litterfall fluxes with each as an independent dataset. Moreover, these variables may be measured multiple times during a long-term study, but not necessarily at the same time or at the same frequency. Finally, information from a single site may include a gradient study across a hillslope, chronosequence, or region that may influence how data users want to aggregate individual measurements. The SoDaH metadata template prompts data providers to indicate if data from multiple files need to be aligned, and, if so, the grouping variable(s) that can be used to join this information. The template also prompts data providers to indicate if datasets include time-series data or data from a gradient study. Users of SoDaH are encouraged to consider this information in their analyses.

3 Database description

3.1 Spatial and temporal distributions

The SoDaH database currently contains data from 215 locations and 186 unique study sites, with data contributed from DIRT, NutNet, LTER, NEON, and CZO networks. There are more locations than study sites in the database because some sites contributed datasets from multiple locations or experiments. The flat database contains 160 columns of variables and nearly 300,000 rows of information, but is relatively sparsely populated, with 13.9 million non-missing observations (roughly 30% of the database). Given the focus on NSF funded research networks and observatories, most of the measurements are taken from the United States, but NutNet and DIRT networks include a number of international study sites (Fig. 4).

Mean annual temperature from all locations was 10.1 ± 7.1 °C (mean ± 1$\boldsymbol{\sigma}$, n = 212) with a range of -12 to 27.2 °C. Mean annual precipitation from all locations was 904 ± 638 mm y-1 (n = 213), with a range of 105 to 4250 mm y-1. Land cover classifications include urban, cultivated, rangeland/grasslands, shrublands, and forests, but land cover is reported only for a subset (n = 87) of the study locations.

We briefly review characteristics of data contributed from the five networks represented in SoDaH (Fig. 5). The CZO generally has a focus on making one-time characterizations that extend deeper in soil and regolith profiles than other networks. Data from DIRT spans relatively few sites and only includes surface soil layers, but provides repeated measurements and their response to experimental manipulations. The LTER network provides data from comparatively few study sites, but LTER sites have longer measurement records than other networks in SoDaH given the network’s 40-year history. Some data from LTER

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sites also include measurements to ~1m depth. By design, NEON provides data with broad geographic coverage and samples both surface and deeper soil horizons. The current temporal record from NEON sites is relatively short, but is expected to extend for the next 30 years. Finally, NutNet provides the greatest number and largest spatial distribution of sites, all from grassland ecosystems with sampling depths from 0 to 10 cm.

3.2 Experimental manipulations, gradients, and time series

SoDaH is unique in the landscape of soil databases because it includes data from both experimental manipulations (at 132 sites) and gradient studies, and includes time series of soil data. Nutrient manipulations from NutNet make up the majority (109) of experimental manipulations. All experimental manipulations in SoDaH are summarized in Table 1, and include manipulations from all fifteen LTER sites for which we have data, six DIRT sites and one CZO site. The database also includes gradient studies from 66 sites (with data from NEON, CZO and LTER networks), and time series data from 158 sites (with data from NutNet, NEON, LTER, and DIRT networks, Table 1).

3.3 Database use and analyses

Aggregating data in SoDaH presents challenges in how to most appropriately group multiple measurements taken from individual study locations that include diverse sampling protocols, unique experimental designs, and measurements from multiple soil depths. Moreover, particular locations may include manipulative experiments, gradient studies, and time series of repeated measurements. The appropriate aggregation of SoDaH requires users to become familiar with data structures of the database to address particular scientific questions. For this reason, we see the RShiny web-app as an invaluable tool for querying the data available from SoDaH. As mentioned in section 2.4, future contributions to the LTER SOM GitHub repository should focus on developing additional utilities to align and aggregate datasets from individual sites and locations.

3.4 Database contributions and database versioning

We built the SoDaH tools to help facilitate the harmonization of diverse soils datasets that focus on soil C. Towards that end, we welcome contributions of new data from new sites that may be part of the research networks presented here, additional research networks (e.g. Ameriflux https://ameriflux.lbl.gov/, Drought-Net https://wp.natsci.colostate.edu/droughtnet/, Long-Term Agroecosystem Research https://ltar.ars.usda.gov, African soils database http://africasoils.net/services/data/, European LTERs https://www.lter-europe.net/, or others), as well as data from sites that are unaffiliated with a research network. The SoDaH website (https://lter.github.io/som-website/database.html, last accessed July 15, 2020) contains more information on how to contribute data. Briefly, data contributors need to place raw datasets and a completed copy of the SoDaH metadata template into a shared Google Drive folder and notify the SoDaH editor (soildataharmonization@gmail.com) that their data are ready for ingestion into SoDaH. We ask that new contributions of Level 0 data that are harmonized into SoDaH be published with a unique DOI.

Updated releases of SoDaH will be made periodically after a threshold number of new contributions have been made to the database, in light of any changes to the database structure, or if any errors are detected and corrected. Versions are tracked with a version number in the form of "major.minor." in addition to the date of publication. Each version of the dataset will receive a unique citation and DOI through the EDI data portal for users to reference.

4.0 Data availability and user guidelines

The SoDaH v1.0 database and some exemplary analyses are hosted in the EDI repository (Wieder et al., 2020; https://doi.org/10.6073/pasta/9733f6b6d2ffd12bf126dc36a763e0b4 accessed 15 July 2020). We encourage users of SoDaH data to cite both this publication and the dataset citation provided by the EDI data portal in their products.

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Table 1. Summary of the networks and number of sites contributing data from experimental manipulations, gradient studies, and time series of repeated measurements

Experimental Manipulation	**Networks (site)**
Nutrient additions	NutNet (109) LTER (5)
Litter manipulations	DIRT (6)
Agricultural management	LTER (3)
Forest harvest	LTER (2) CZO (1)
Warming	LTER (2)
Fire	LTER (2)
Precipitation manipulation	LTER (2) CZO(1)
Elevated CO_2	LTER (1)
Other (mostly related to management, disturbance, or land use history)	NutNet(109) LTER (10) CZO (1)
Gradient Studies	NEON (47) LTER (11) CZO (7)
Time Series	NutNet(109)^ NEON (35)§ LTER (10) DIRT (5)

^ Repeated measurements for NutNet are for plant productivity, not soil measurements
§ Not all NEON sites have been sampled more than once per dataset

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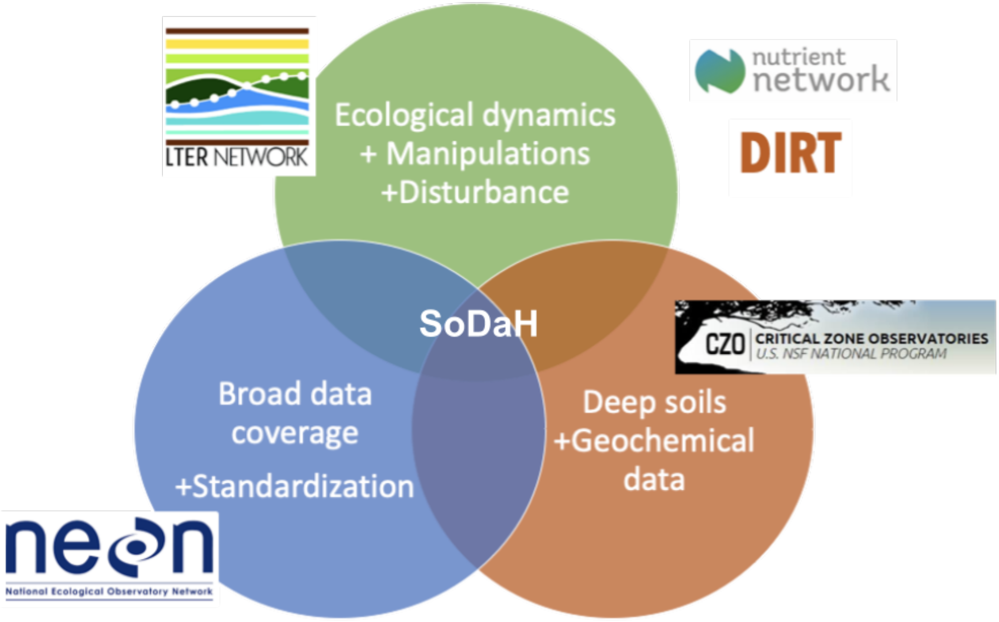

Figure 1: Conceptual diagram that summarizes the strengths and research foci of different experimental networks contributing to SoDaH, modified from Weintraub et al. 2019.

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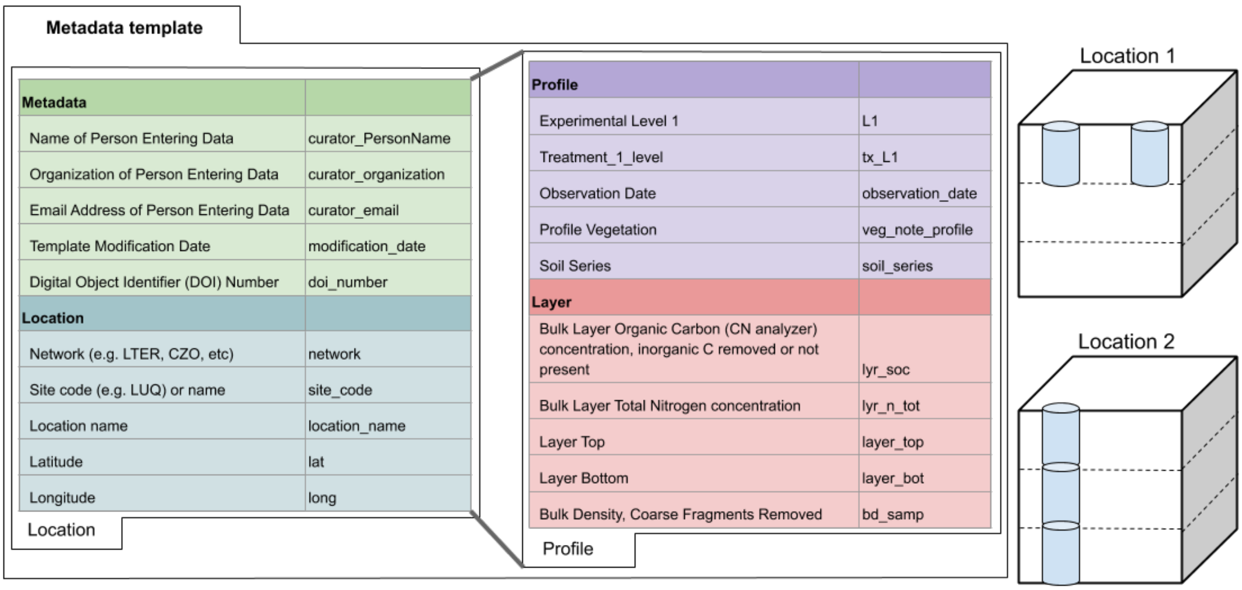

Figure 2: Diagram showing hierarchical relationship between data fields in the Soils Data Harmonization (SoDaH) database, which includes metadata, location, profile and layer fields. Each data field lists a short description of some of the variables used along with the variable name used in the database. To facilitate data contributions these data fields were grouped into Location and Profile tabs on the metadata template used by data contributors. As an example, Location 1 provides data from two profiles that each have information from one layer, whereas Location 2 provides data from one profile that has information from three layers. Any location may provide data from multiple profiles or layers.

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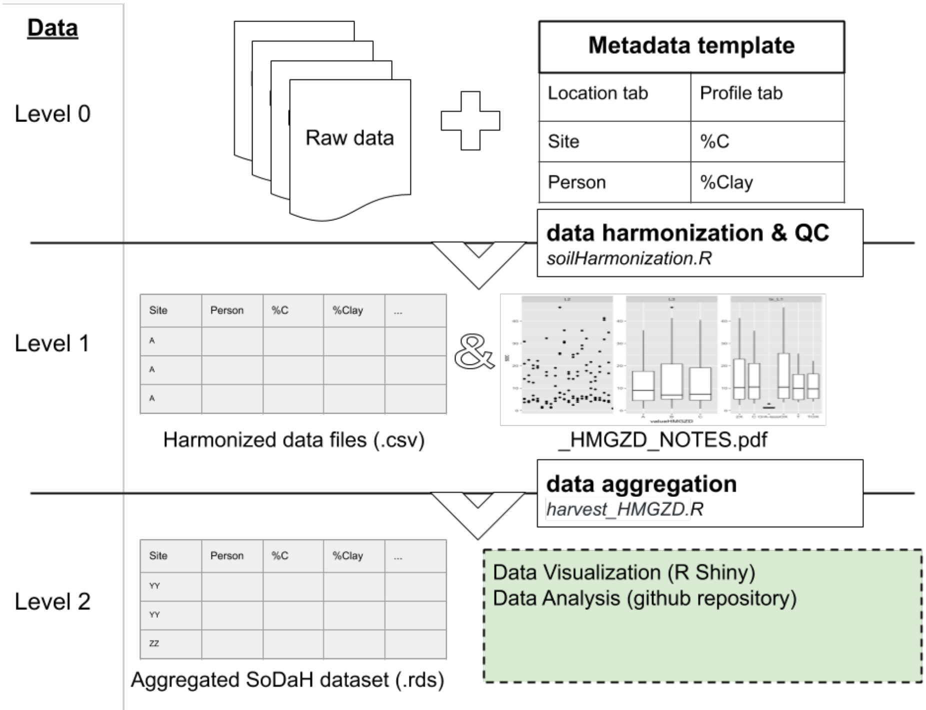

Figure 3: Illustration of the SoDaH workflow and data levels. Raw data (Level 0) are identified by data providers and variables are mapped to standardized units and vocabulary using the metadata templates. These data are homogenized into Level 1 data with soil harmonization script that renames variables, conducts unit conversions, and performs quality control checks. Finally, Level 1 data are aggregated into the Level 2 dataset, which can be visualized with the SoDah R Shiny app and queried with data analysis tools.

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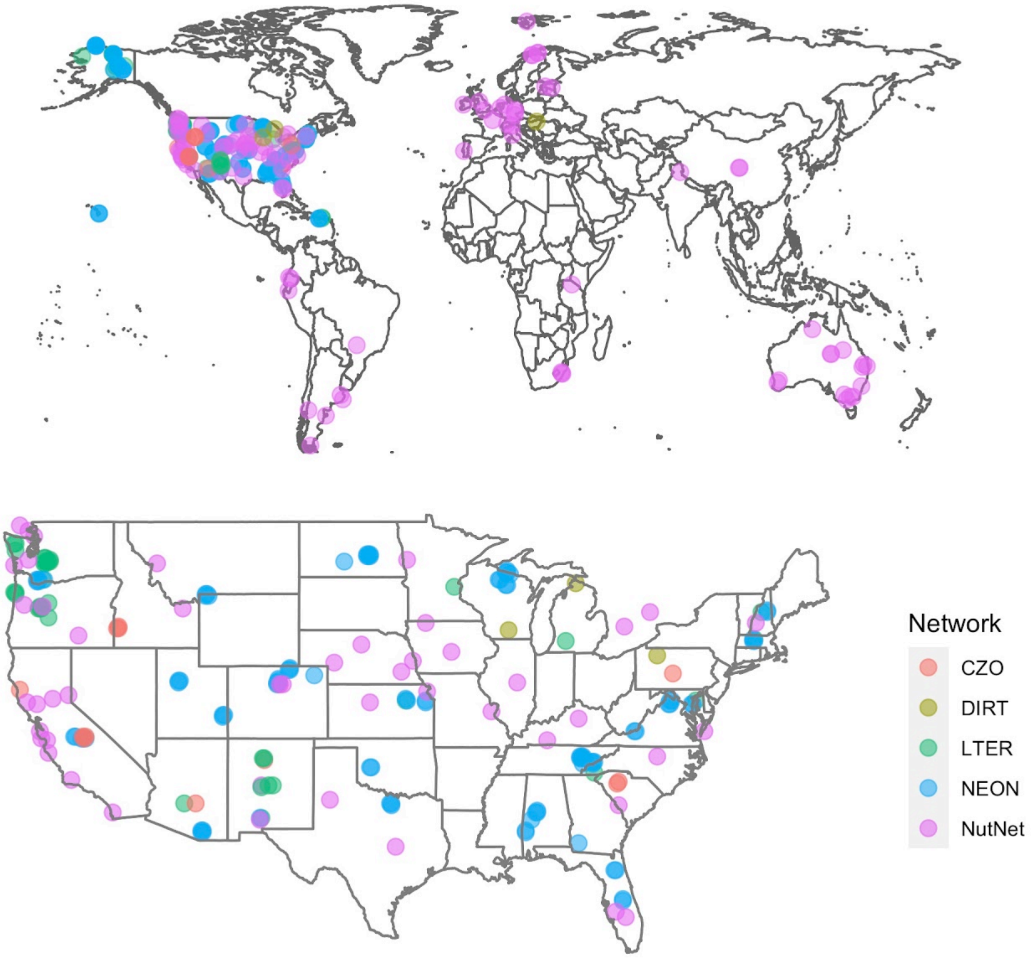

Figure 4: Spatial distribution of study locations representing five research networks in SoDaH globally and in the contiguous USA.

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Figure 5: Temporal coverage and depth of measurements taken from different study sites and grouped by research network.