Data From: TERRA-REF, An Open Reference Data Set From High Resolution Genomics, Phenomics, and Imaging Sensors

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Abstract

The ARPA-E funded TERRA-REF project is generating open-access reference datasets for the study of plant sensing, genomics, and phenomics. Sensor data were generated by a field scanner sensing platform that captures color, thermal, hyperspectral, and active flourescence imagery as well as three dimensional structure and associated environmental measurements. This dataset is provided alongside data collected using traditional field methods in order to support calibration and validation of algorithms used to extract plot level phenotypes from these datasets.

Data were collected at the University of Arizona Maricopa Agricultural Center in Maricopa, Arizona. This site hosts a large field scanner with fifteen sensors, many of which are capable of capturing mm-scale images and point clouds at daily to weekly intervals.

These data are intended to be re-used, and are accessible as a combination of files and databases linked by spatial, temporal, and genomic information. In addition to providing open access data, the entire computational pipeline is open source, and we enable users to access high-performance computing environments.

The study has evaluated a sorghum diversity panel, biparental cross populations, and elite lines and hybrids from structured sorghum breeding populations. In addition, a durum wheat diversity panel was grown and evaluated over three winter seasons. The initial release includes derived data from from two seasons in which the sorghum diversity panel was evaluated. Future releases will include data from additional seasons and locations.

The TERRA-REF reference dataset can be used to characterize phenotype-to-genotype associations, on a genomic scale, that will enable knowledge-driven breeding and the development of higher-yielding cultivars of sorghum and wheat. The data is also being used to develop new algorithms for machine learning, image analysis, genomics, and optical sensor engineering.

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Introduction

General information

• Title: TERRA-REF, An Open Reference Data Set From High Resolution Genomics, Phenomics, and Imaging Sensors

- Dates of Data Collection: 2017 and 2018
- Geographic Location: Maricopa, Arizona
 - Center of the field: 33.07549° N 111.9749° W
 - Field is approximately 0.4 ha (200 m x 20 m). The scannable area of the field is 22.1 m on East West axis and 205.5 m on N/S axis.
- Keywords: Sensor, Phenomics, Sorghum, TERRA-REF
- Funding: The work presented herein was funded in part by the Advanced Research Projects Agency-Energy (ARPA-E), U.S. Department of Energy, under Award Number DE-AR0000598. Computational support was provided by the National Center for Supercomputing Applications and XSEDE.

The data pipeline used to process sensor data and generate derived data was described in the Burnette et al. (2018) ACM PEARC 2018 proceedings paper "TERRA-REF data processing infrastructure".

Data Use, Sharing, and Access

To cite this dataset:

LeBauer, D.S., Burnette, M.A., Demieville, J., Fahlgren, N., French, A.N., Garnett, R., Hu, Z., Huynh, K., Kooper, R., Li, Z., Maimaitijiang, M., Mao, J., Mockler, T.C., Morris, G.S., Newcomb, M., Ottman, M., Ozersky, P., Paheding, S., Pauli, D., Pless, R., Qin, W., Riemer, K., Rohde, S., Rooney, W.L., Sagan, V., Shakoor, N., Stylianou, A., Thorp, K., Ward, R., White, J.W., Willis, C., and Zender C.S. 2020. TERRAREF, An Open Reference Data Set From High Resolution Genomics, Phenomics, and Imaging Sensors. Dryad Digital Repository. http://doi.org/10.5061/dryad.TBD

This data publication consists of data and metadata, as described below. Plot level phenotypes, experimental meta-data, and a catalog of large files are available on Dryad. The file catalog provides the location of larger sensor files that can be accessed using the Globus file transfer service.

Because the dataset contains over 400TB of sensor data files, these large files are stored at the National Center for Supercomputing Applications and are made available using the Globus file transfer service.

In addition to hosting an archival copy of data on Dryad, the documentation includes instructions for browsing and accessing these data through a variety of online portals. These portals provide access to web user interfaces as well as databases, apis, and R and Python clients. In some cases it will be easier to access data through these portals using web interfaces and software libraries.

Except where clearly indicated for sensor data, the structure of directories that contain data and metadata refer to the contents of the Dryad archive. There are four directories: data, metadata, code, and documentation.

The TERRA-REF documentation is hosted at docs.terraref.org. The section "How to Access Data" provides an overview of methods that can be used to access data beyond what is provided in this repository. There is also a PDF copy of the documentation in the file docs.terraref.org_2020_04_06.pdf in the metadata/directory.

Tutorials for getting started with TERRA-REF data are available at terraref.org/tutorials and on GitHub at github.com/terraref/tutorials.

The TERRA-REF YouTube channel hosts 1) video walkthroughs of the tutorials https://www.youtube.com/channel/UComeQAqYR5aZrXN_3K5iFGw and 2) a playlist of videos related to the project https://www.youtube.com/playlist?list=PLNgRX4VLed8213stlJp60MvVx2p6VTv6N.

All data are released to the public domain under the CC-0 license. All original software are licensed with the BSD 3-clause or MIT/BSD compatible license. All software used for data processing have been archived on Zenodo and are available on GitHub in the terraref organization: github.com/terraref.

This software was created specifically for the field scanner data processing pipeline that is described by Burnette et al. (2018). The file code/source_code_dois.txt provides the DOIs for code archives that contain the state of the software at the time the data were processed.

Component	Github Organization / Repository	Archive Citation
TERRA-REF Documentation	terraref/documentation	LeBauer et al. (2020b)
Reference Data	terraref/reference-data	LeBauer et al. (2020a)
Sensor Metadata	terraref/sensor-metadata	Willis et al. (2020)
Computing Pipeline	terraref/computing-pipeline	Burnette et al. (2020)
terrautils Python Library	terraref/terrautils	Burnette et al. (2019e)
Metadata Processing	terraref/extractors-metadata	Burnette et al. (2019c)
Laser 3D Scanner	terraref/extractors-3dscanner	Burnette et al. (2019f)
Environmental Logger	terraref/extractors-environmental	Burnette et al. (2019d)
Hyperspectral	terraref/extractors-hyperspectral	Mao et al. (2019)
Multispectral, Thermal, PSII	terraref/extractors-multispectral	Burnette et al. (2019a)
Stereo RGB	terraref/extractors-stereo-rgb	Burnette et al. (2019b)

Other Software used in this project:

Software	Github Organization / Repository	Software Archive	
Clowder	clowder-framework/clowder	Marini et al. (2019)	
BETYdb Trait Database	pecanproject/bety	Rohde et al. (2016)	

Datasets

In this README, we define the following types of data:

- 1. **Sensor Data** from five thermal, light, and shape imaging sensors scanning a 4000 m² field at hourly to weekly intervals at 1 mm² scale resolution. Additional details in the section on sensors and sensor technical descriptions that can be found in the metadata/sensors/ directory of this repository.
- 2. **Phenotypes** include both sensor-derived and standard field measurements required to validate and calibrate algorithms that compute plant phenotypes from remote sensing data.
- 3. Environmental data include time series of meteorological variables including temperature, relative humidity, precipitation, wind direction and speed, photosynthetically active radiation, and downwelling spectral radiance.
- 4. **Genomics** data include whole-genome resequencing data for 384 varieties from the sorghum Bioenergy Association Panel (BAP) and genotyping-by-sequencing data for 768 sorghum Recombinant Inbred Lines (RILs). Contains raw and derived sorghum genome sequencing data. Raw data includes DNA sequence files in compressed FASTQ format. Derived data are available in Variant Call Format (VCF) and Hapmap files.

Sensor Data

Field Scanner Sensors

This publication includes the following data generated by sensors. Detailed sensor and system details can be found in the file metadata/sensors_information.zip as well as browsed online through the Clowder Interface terraref.org/clowder in a space named "Maricopa Agricultural Center Device and Sensor Information".

The sensor information folder contains extensive documentation for each of the sensors, the field scanner, calibration targets, and the results of sensor validation tests.

Additional sensors not represented in this version of the data are listed in the section on sensors in the section on additional sensors.

Sensor Name	Model	Technical Specifications
Imaging Sensors		
Stereo RGB Camera	Allied Vision Prosilica GT3300C	
Laser Scanner	Custom Fraunhofer 3D)	Spatial Resolution: 0.3 to 0.9 mm
Thermal Infrared	FLIR A615)	Thermal Sensitivity $< 50 \text{mK}$ @ 30°C
PS II Camera	LemnaTec PS II Fluorescence Prototype)	Illumination 635nm x 4000 μ mol/m ² /s, Camera 50 fps
Environmental Sensors	,	. , , , ,
Environmental Sensors	Thies Clima 4.9200.00.000)	
VNIR Spectrometer	Spectral Evolution PSR+3500	Range 350 to 800 nm
Environmental Sensors	Thies Clima 4.9200.00.000)	
VNIR Spectrometer	Spectral Evolution PSR+3500	Range 350 to 800 nm
PAR Sensor	Quantum SQ-300	Spectral Range 410 to $655~\mathrm{nm}$

Sensor Data Products

The total size of raw (Level 0) data generated by these sensors is 60 TB. Combined, the Level 1 and Level 2 sensor data products are 490 TB. This size could be substantially reduced through compression and removal of duplicate data. For example, the same images at the same resolution appear in the georeferenced Level 1 files, the full field mosaics, and the plot level clip.

Sensor data are stored on the Storage Condo at the National Center for Supercomputing Applications in Urbana, Illinois. We make them available for download with the Globus file transfer system. The following steps are required to access them: 1) get an account at globus.org; 2) search for the terra-public endpoint; 3) install the Globus Personal Connect application and transfer data. Further information is provided in the data access chapter of the TERRA-REF documentation. As an alternative, the data can be provided on hard drives for the cost of supplies, labor, and shipping.

Sensor Data Catalog

Globus provides the easiest way to navigate the data. This archive also contains a catalog listing all of the files in the dataset. The catalog is one compressed .zip file per season, currently seasons 4 and 6, found in the data/ directory in files named season_[n]_catalog.zip. The compressed catalogs are 373 MB total, and expand to 5.4 GB when uncompressed. After uncompressing the catalog files, the catalog contains one directory per data product and one file per day named [data product]/file_catalog_season[n]_[data product]_[filetype]_[YYYY-MM-DD].json.

These catalog files contain the following information in JSON format:

```
collections: 'collection name [Data Product Name] - [YYYY-MM]'
  datasets: 'dataset name [Data Product Name] - [YYYY-MM-DD]'
  files:
     path: 'season-[n]/Level_[m]/[data_product]/[filename]'
     checksum: '[checksum_string]'
     name: '[data product]_L[m]_[YYYY-MM-DD]_[Scan Name]'
     size: 'bytes'
```

There is one collection per data product per month, and one dataset per data product per day. This structure of collections and datasets refers to the organization of files in the the Clowder database and web interface see data access documentation.

Below is a summary of the sensor data products included in the first release of TERRA-REF data. Sensor-derived phenotypes described in the Phenotype Data section were generated from the 3D laser scanner and RGB camera sensors as described in the file metadata/methods.csv.

Data Product	Sensor	Algorithm	File Format	Plot Clip	Full Field
Environment	Thies Clima	envlog2netcdf	netcdf	NA	NA
Thermal Image	FLIR	$ir_geotiff$	geotiff	+	
Point Cloud	Fraunhofer Laser 3D	$laser3d_las$	las	+	
Point Cloud	Fraunhofer Laser 3D	scanner 3D Top	ply		
Images Time-Series	PSII Camera	ps2png	png		
Color Images	RGB Stereo	bin2tiff	geotiff	+	+
Plant Mask	RGB Stereo	rgb_mask	geotiff		X

Figure 1 shows the number of files for each data type across seasons 4 and 6.

Sensor Data Directory Contents

The following list describes the organization and contents of the Storage Condo server. These can be accessed at the ncsa#terra-public endpoint on Globus. Directory names have a leading / while file names do not.

• Environment Logger

- /envlog netcdf
 - * Daily aggregated files named envlog_netcdf_L1_ua-mac_[YYYY-MM-DD].nc.
 - * There are also 24 hourly files for each day named [YYYY-MM-DD_HH-MM-SS]_environmentlogger.nc.

• Laser3D

- /laser3d las
 - * One merged file per scan across the short (E-W) axis with names ending in _merged.las. There are typically 50-100 of these each day.
- /laser3d_las_plot
 - * Each directory has the name of one plot, and there is one LAS file clipped to the plot boundaries for each scan (there may be more than one scan per day).

• RGB Stereo:

- /rgb_geotiff
 - * File names ending in _left.tif and _right.tif represent simultaneous images from left and right stereo pair cameras.
- /rgb mask
 - * These images have the soil represented as black pixels. For each file ending in *_left_mask.tif in the RGB Geotiff dataset, an image with black pixels representing areas that contain soil and not plants.

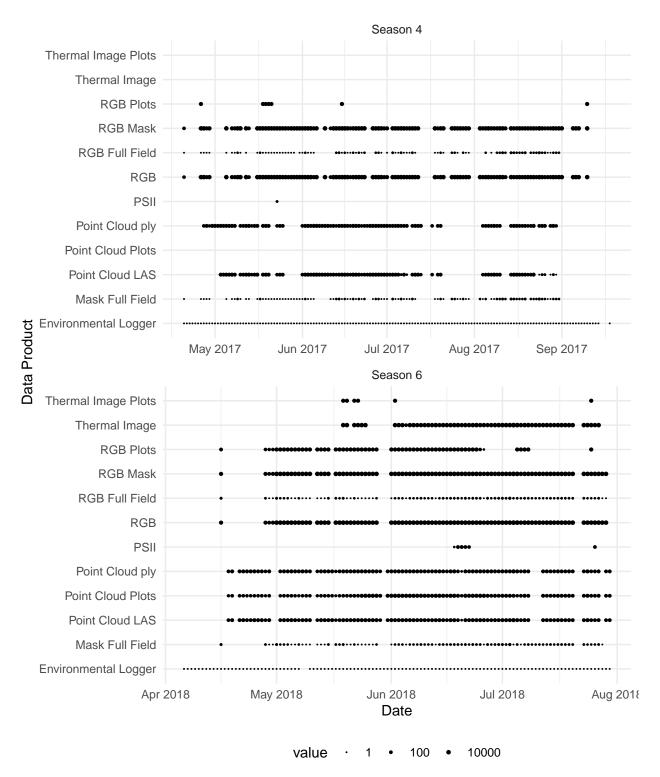


Figure 1: Counts of individual files for each type of sensor data product.

- /rgb_geotiff_plots

* For each RGB Geotiff image, a Geotiff file with the same dimensions as the plot. It contains the image clipped to the plot boundaries as well as fill values for parts of the plot not in the image.

- /rgb_fullfield

- * Key data product is one full resolution full-field image per scan.
- * Other files include: lower resolution versions of the full field (files with names ending in _10pct.tif, _thumb.tif and .png); CSV files containing canopy cover values for each plot; a JSON file listing images contained in the fullfield mosaic; a VRT file that is a "virtual geotiff" that was used to generate the full-field mosaic.
- * These full field Geotiff images are RGB images and image masks tiled together to make up a full-field view. These full field images are *not* orthomosaics since they are not stitched together because doing so causes geometric aberrations.

• PSII Camera:

- /ps2_png:
 - * 101 .png files per folder. The order of the images is indicated by the last four digits of the file name, i.e. _0000.png to _0100.png.
 - * 101 georeferenced Geotiff files otherwise identical to the PNG counterparts.
 - * These files represent a time series of images captured at a rate of 50 frames per second.

Sensor Data Directory Structure and File Naming

File names follow consistent patterns based on data product and date of collection. These are intended to be easily understood. The hierarchy is season, data product level, date, date-time, and files.

Specifically, under the directory /season-[4,6] we have:

```
|-Level
| |- Data product name
| | |-Date (YYYY-MM-DD)
| | | |-Date-Time (YYYY-MM-DD__HH-MM-SS-SSS)
| | | | | - File name(s)
|-Level_1
| |- envlog_netcdf
| | |-2017-08-26
| | | |-2017-08-26_13-34-54-321_environmentlogger.nc
| |- laser3d_las
| | |-2017-08-26
| | | |-2017-08-26_12-34-54-321
| | | | scanner3DTop - 2017-08-26_12-34-54-321 MergedPointCloud.las
```

For convenience, we have pre-processed some images and point clouds to plot boundaries and have organized them by Date and then Plot name, e.g.:

```
|-Level_1_plots
| |- rgb_geotiff
| | |- 2017-04-26
| | |- MAC Field Scanner Season 4 Range 21 Column 16
| | | |- rgb_geotiff_L1_ua-mac_2017-04-26__12-56-14-907_right.tif
| | | |- rgb_geotiff_L1_ua-mac_2017-04-26__12-56-14-907_left.tif
| | | |- rgb_geotiff_L1_ua-mac_2017-04-26__12-53-34-106_right.tif
```

Phenotype Data

Raw Phenotype Data

Tables of phenotypes can be found in the compressed files data/season_4_traits.zip and data/season_6_traits.zip. Once uncompressed, each directory will contain one CSV file for each combination of trait and measurement method. The names of these CSV files help identify the contents because they follow the pattern season_[n]_[trait]_[measurement_type].csv. For example, the file season_6_aboveground_biomass_manual.csv contains manual measurements of above-ground biomass taken during season 6. Figure @ref(fig:trait_counts) provides a summary of available traits and the dates on which they were collected.

These CSV files have one measurement per row for a specific date, location, genotype, and measurement. The first line is a header that contains the names of the fields:

- plot (text) Plot name, using the format <field site> Season <n> Range <m> Column <k>.
- scientificname (text) Latin name for the crop species. This will always be *Sorghum bicolor* until future versions with data from additional crops are published.
- genotype (text) Genotype or accession identifier.
- treatment (text) Name of experimental treatment.
- date: (YYYY-MM-DD) Date of measurement.
- trait: (text) Name of the trait measured. Defined in the file metadata/variables.csv.
- method: (text) The method used to measure the trait. Defined in the file metadata/methods.csv.
- mean: (numeric) Value of the phenotype data.
- checked: (boolean) 0 = unchecked and 1 = checked: has the data been independently reviewed?
- author: (text) name of scientist who collected the data or who wrote the algorithm used to derive phenotypes from sensor data.
- season: (text) Name of season: one of 'Season 4' or 'Season 6'.
- method_type: (text) Type of measurement: one of 'manual' or 'sensor'.

Code

For the purposes of reproducibility, the code used to run and query data from a copy of the TERRA REF trait database terraref.org/bety is provided. This uses Docker to run the database and R to query the data and prepare the CSV files. The code/ directory contains the following:

- An R script s4s6_sql2csv.R that connects to the database and generates the phenotype data files described above. This requires a copy of the database. Instructions for installing the database using Docker are found in betydb_docker. A much slower implementation that uses the API and the R traits package Chamberlain et al. (2019) is provided in code/s4s6_slow_api.R.
- The betydb_docker/ folder that contains files named Docker, docker-compose.yml, README.md and .pgpass. This allows a user to run a copy of the TERRA REF PostgreSQL database containing phenotype data and agronomic metadata. Instructions are in the README.md file and database connection parameters are in the .pgpass file. This database can be queried using the included R script or from any programming language using the credentials stored in the .pgpass file.

Environmental Data

Weather

We have data from two stations, AZMet and the field scanner system.

Field Scanner System "Environment Logger"

These data are from the Theis-Clima weather station mounted on the field scanner. The Environment Logger has more sensors and provides high temporal resolution data than the weather station. In the NetCDF files, data is recorded at five seconds intervals. This logger also collects the downwelling solar radiation every five seconds at a spectral resolution of 0.5 nm. The sensors and data collection frequency are described in the section on sensor data. We describe both the full resolution data provided as NetCDF files in the sensor data product named "envlog_netcdf" and the 5-minute aggregated data provided here as JSON files that were accessed using the Geostreams API as described in the TERRA REF tutorials. These time series are not continuous, as can be seen in Figure 3.

Environment Logger Aggregated JSON Files

The files metadata/weather/envlog_aggregated/season_[n]_envlog.json were downloaded from the Geostreams API on April 21 2020. The API is described in the tutorials, and the specific calls used to download these files are in code/envlog_curl.sh.

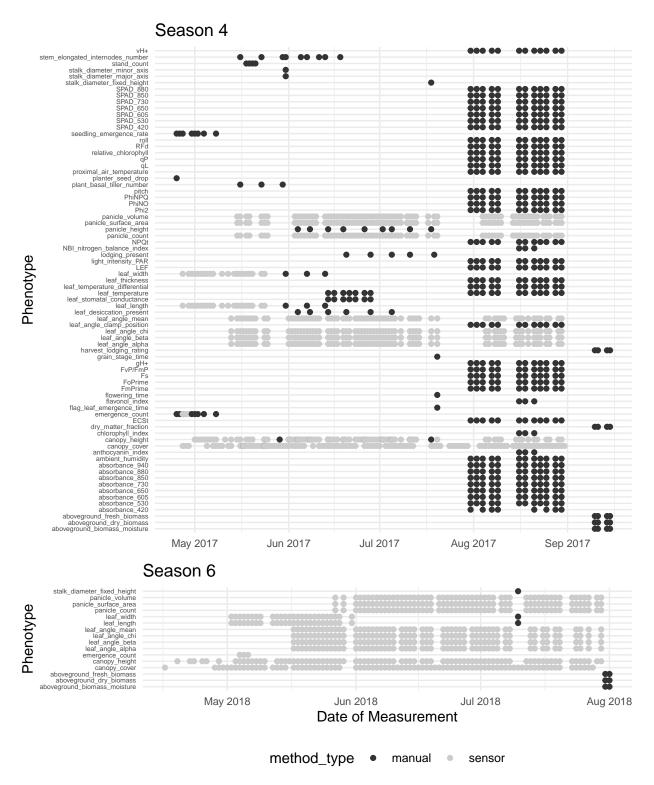


Figure 2: (#fig:trait_counts)Counts of individual plot level measurements for each trait.

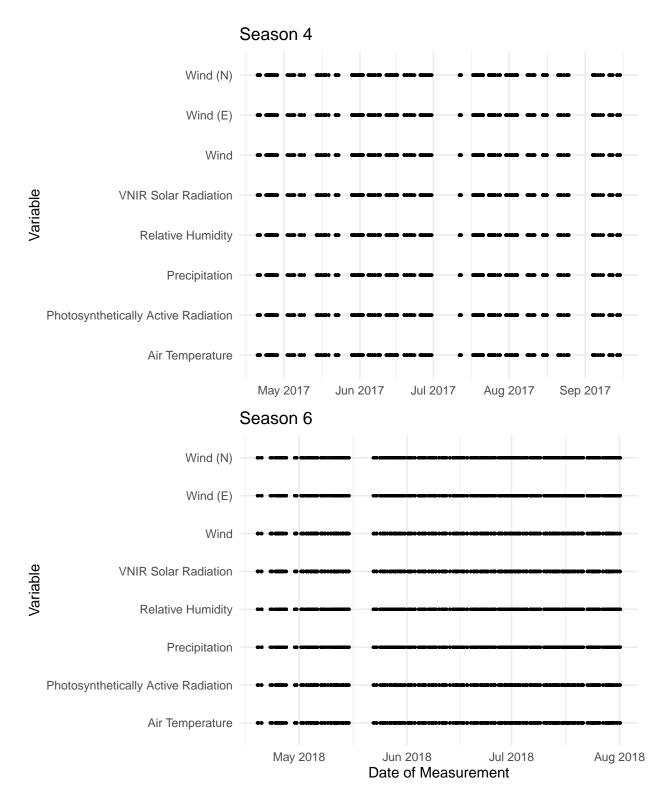


Figure 3: Dates of aggregated weather data - available through the Geostreams API and in the metadata/weather folder.

Environment Logger NetCDF Files

These are even higher resolution time series.

The files for each season are approximately 40 GB and, like sensor data, are provided using methods such as Globus transfer or the Clowder API (see "How To Access Data" in the documentation). On Globus, they are in the /ua-mac/Level_1/envlog_netcdf/ directory.

The data are described in the TERRA REF documentation under the environmental data section of the data products chapter.

The primary reason that these files are so large is that they contain the downwelling spectral radiance measurements (350-800 nm) at five second intervals.

On Globus, each date will include hourly files named [YYYY-MM-DD_HH-MM-SS]_environmentlogger.nc and as a single daily file named envlog_netcdf_L1_ua-mac_[YYYY-MM-DD].nc. The daily file contains all of the hourly files concatenated into a single file for ease of use.

AZMET

These gap-filled and corrected data have been provided for convenience. When using these data, **users must cite** Brown and Russell (1996): > Brown, P. W., & Russell, B. (1996). AZMET, The Arizona Meteorological Network. Arizona Cooperative. website: https://cals.arizona.edu/AZMET/.

Both hourly and daily values are available, and can be found in the /metadata/weather/azmet folder of the Dryad repository. There are four CSV files – one daily and one hourly for each season, and a README file that provides a description of their content. These files have not been modified from the collection on the website other than to subset it to the time range of the two seasons of sensor and phenotype data.

Soils Data

A comprehensive analysis of soil physical properties will be published alongside the TERRA-REF datasets (Babaeian et al., 2020).

Genomics Data

The Biomass Association Panel planted in Seasons 4 and 6 was described by Brenton et al. (2016). These genotypes have been sequenced and the sequence data and SNPs are provided as an archive on Dryad. A copy of these data is available on the CyVerse Data Store https://datacommons.cyverse.org/browse/iplant/home/shared/terraref.

The genomics dataset includes raw and derived sorghum genome sequencing data from the TERRA-REF project. Raw data includes DNA sequence files in compressed FASTQ format. Derived data is available for whole-genome resequencing and genotyping-by-sequencing.

These data are archived in the same filesystem as the sensor data, and available at the Globus ncsa#terra-public endpoint under the genomics/ directory. A copy is available in the CyVerse data store.

At both Globus and CyVerse, the data is organized in the following directory structure:

```
|-terraref
| |-genomics
| | |-raw_data
| | | |-bap
| | | |-resequencing
| | | |-ril
```

Germplasm

A list of cultivars and the experiments in which they are planted are listed in the file metadata/germplasm.csv.

The germplasm.csv file contains the following fields:

- germplasmName Genotype identifier used by TERRA REF; typically equal to Genesys Accession Number
- germplasmPUI UUID from Genesys
- season_4 A boolean which is TRUE if the accession was planted in Season 4 experiments.
- season_6 A boolean value which is TRUE if the accession was planted in Season 6 experiments.

For user convenience, we also provide this information and additional metadata in a format that follows the Breeder's API (BrAPI) specification v1.3 Selby et al. (2019) in files named season_[n]_germplasm.json and in the terraref_sorghum_bap_samples.txt table alongside raw sequencing data (described below).

Whole-genome resequencing data for the sorghum Bioenergy Association Panel (BAP)

Raw data

There are 384 available samples. Each sample is stored as a pair of files in bzip2 FASTQ format with names ending in *_R1.fastq.bz2 and *_R2.fastq.bz2. R1 and R2 in these names represent read pairs one and two. Each file in a pair has the same number of DNA sequences that line up and are read from opposite ends of the same sequenced molecule.

A table of sample information (terraref_sorghum_bap_samples.txt) can be found in the raw data directory genomics/raw_data/bap/resequencing.

Each table contains the following fields:

- identifier: The unique genotype identifier that will be used in the derived data outputs
- accession: Genotype identifier used by TERRA REF
- taxid: Taxonomy identifier from the NCBI taxonomy database
- organism common name: Genbank common name from the NCBI taxonomy database
- subspecific genetic lineage rank: Cultivar
- subspecific genetic lineage name: Unique germplasm identifier
- ploidy: Source, Phytozome
- number of replicons: Number of chromosomes, source Phytozome
- estimated size: Estimated genome size, source Phytozome
- source material identifiers: UUID from Genesys
- sample name: Internal sample identifier
- raw file 1: File name for read-pair 1
- raw file $\mathbf{2}$: Filename for read-pair 2

Derived data

Data derived from analysis of the raw resequencing data at the Danforth Center (version1) are available as gzipped, genotyped variant call format (gVCF) files and the final combined hapmap file in the derived data directory, genomics/derived_data/bap/resequencing/danforth_center/version1.

Genotyping-by-sequencing (GBS) data for sorghum recombinant inbred lines (RIL)

Raw data

Raw data are in gzip FASTQ format. There are 768 available samples.

A key file (Key_ril_terra) with sample information can be found in the raw data directory, genomics/raw_data/ril/gbs.

Derived data

Combined genotype calls are available in VCF format in the derived data directory, genomics/derived_data/ril/gbs/kansas_state/version1.

Future Releases

For the first public release of data we have focused on a subset of the data that we collected, processed, and subjected to quality assurance and control. We expect that this initial data release and subsets of these data curated for specific research projects will provide users and funders with sufficient information to justify processing, validating, and storing data from additional seasons and sensors.

Here we provide a description of additional data that can be made available for future use.

This data release does not contain all of the data that was collected during the TERRA-REF project. The field scanner was operated as part of the TERRA-REF program with the mission of generating open access data from April 2016 to September of 2019. Although this release focuses on two seasons of data, the first priority is to make all of the raw data and metadata is available in the public domain. This raw data archive is in the process of being transferred to tape-storage at the Texas Advanced Computing Center and we expect it will be available in late 2020.

Additional derived products from the project are also available for use, but are not in the public domain because they have not been consistently curated, processed, and validated. These data are available for use - researchers interested in using these data or creating new datasets are invited to contact the authors for more information. The primary constraint on processing and publishing these datasets is the availabilty of scientists and engineers to process and validate the data.

Any use of these unpublished derived datasets must adhere to the data use and authorship guidelines outlined in the TERRA-REF documentation at docs.terraref.org and the file documentation/docs.terraref.org_2020_04_06.pdf.

Additional Sensors Not Included in the Current Data Release

At this point we have not sufficiently validated data or curated data from the following sensors. For the VNIR and SWIR hyperspectral imaging cameras this reflects challenges faced in calibration. Other sensors have not been prioritized.

Sensor		
Name	Model	Technical Specifications
Multi- spectral Ra- diome-		
ters Dedicated NDVI Multispectral	Skye Instruments SKR $1860D/A$	650 nm, 800 nm +/- 5 nm; 1 down, 1 up
Radiometer Dedicated PRI Mul- tispectral Radiometer	Skye Instruments SKR 1860ND/A	531nm +/- 3nm; PRI = Photochemical Reflectance Index
Active Reflectance	Holland Scientific Crop Circle ACS-430	$670~\rm{nm},730~\rm{nm},780~\rm{nm}$
VNIR Spectroradio	Ocean Optics STS-Visometer	Range: 337-824 nm @ 1/2 nm
Hyper- spectral Cameras		
VNIR Hyper- spectral	Headwall Inspector VNIR	$380\text{-}1000~\mathrm{nm}$ @ $2/3~\mathrm{nm}$ resolution
Imager SWIR Hyper- spectral Imager	Headwall Inspector SWIR	900-2500 nm @ 2/3 nm resolution
Environme	ental	
SWIR	Spectral Evolution PSR+	Range $800-2500$ nm; Installed 2018
Spectromete		
Open Path CO ₂ Sensor	Vaisala CARBOCAP Carbon Dioxide Probe GMP343	Range: 0-1000 ppm

Additional Seasons Not Included in the Current Data Release

Crop			Planting	
Стор	Experiments	Populations ¹	Date	Harvest
Sorghum	Density	BAP, RIL	2016-04-20	2016-07-
				16
Sorghum	Uniformity Trials ²	Stay Green RILs F10	2016-07-27	2016-12-
				02
Durum		Diversity Panel	2016-12-15	2017-04-
Wheat				05
Sorghum	Late Season		2017-04-13	2017-09-
	Drought			21
Durum		Diversity Panel	2017-11-20	2018-04-
Wheat				05
Sorghum		BAP	2018-04-20	2018-08-
				02
Sorghum	Hybrid Uniformity	Stay Green RILs, Mutants, F2	2018-08-23	2018-11-
	Blocks	families		01
Durum	Uniformity Trials	Diversity Panel	2019-01-01	2019-03-
Wheat				31
Sorghum		GRASSL x RIO RILs	2019-05-01	2019-07-
				28
Sorghum		SAP	2019-04-29	2019-09-
				05
	Sorghum Durum Wheat Sorghum Durum Wheat Sorghum Sorghum Durum Corghum Durum Corghum	Sorghum Uniformity Trials ² Durum Wheat Sorghum Late Season Drought Durum Wheat Sorghum Sorghum Hybrid Uniformity Blocks Durum Uniformity Trials Wheat Sorghum	Sorghum Uniformity Trials ² Stay Green RILs F10 Durum Wheat Sorghum Late Season Drought Durum Wheat Sorghum BAP Sorghum Hybrid Uniformity Blocks families Durum Uniformity Trials Diversity Panel Wheat Sorghum GRASSL x RIO RILs	Sorghum Uniformity Trials ² Stay Green RILs F10 2016-07-27 Durum Diversity Panel 2016-12-15 Wheat Sorghum Late Season 2017-04-13 Durum Durum Diversity Panel 2017-11-20 Wheat Sorghum BAP 2018-04-20 Sorghum Hybrid Uniformity Blocks families Durum Uniformity Trials Diversity Panel 2019-01-01 Wheat Sorghum GRASSL x RIO RILs 2019-05-01

 $^{^2 \}rm Uniformity~Trial = same lines planted in strips across field. <math display="inline">^3 \rm In~season~9~a~second~field$ 'North' was added, and separate trials were conducted

Bibliography

- Babaeian, E., Gonzalez-Cena, J. R., Gohardoust, M., Hou, X., White, S. A., and Tuller, M. (2020). Physicochemical and hydrologic characterization terra-ref south field.
- Brenton, Z. W., Cooper, E. A., Myers, M. T., Boyles, R. E., Shakoor, N., Zielinski, K. J., Rauh, B. L., Bridges, W. C., Morris, G. P., and Kresovich, S. (2016). A genomic resource for the development, improvement, and exploitation of sorghum for bioenergy. *Genetics*.
- Brown, P. W. and Russell, B. (1996). AZMET, The Arizona Meteorological Network. Arizona Cooperative Extension.
- Burnette, M., LeBauer, D., Hajmohammadi, S., Li, Z., Willis, C., Qin, W., Patrick, and Maloney, J. (2019a). terraref/extractors-multispectral: Season 6 Data Publication (2019).
- Burnette, M., LeBauer, D., Li, Z., Qin, W., Hajmohammadi, S., Willis, C., Paheding, S., and Heyek, N. (2019b). terraref/extractors-stereo-rgb: Season 6 Data Publication (2019).
- Burnette, M., LeBauer, D., Qin, W., and Liu, Y. (2019c). terraref/extractors-metadata: Season 6 Data Publication (2019).
- Burnette, M., Mao, J., LeBauer, D., Zender, C., and Agrawal, H. (2019d). terraref/extractors-environmental: Season 6 Data Publication (2019).
- Burnette, M., Rohde, G. S., Fahlgren, N., Sagan, V., Sidike, P., Kooper, R., Terstriep, J. A., Mockler, T., Andrade-Sanchez, P., Ward, R., Maloney, J. D., Willis, C., Newcomb, M., Shakoor, N., and LeBauer, D. (2018). TERRA-REF data processing infrastructure. In *ACM International Conference Proceeding Series*.
- Burnette, M., Willis, C., Schnaufer, C., LeBauer, D., Heyek, N., Qin, W., Hajmohammadi, S., and Riemer, K. (2019e). terraref/terrautils: Season 6 Data Publication (2019).
- Burnette, M., Zender, C., JeromeMao, LeBauer, D., Shekar, R., Fahlgren, N., Willis, C., hmb1, Hong, X., ZongyangLi, Wang, F., TinoDornbusch, Maloney, J., Qin, W., Marshall, S., Stylianou, A., and Li, T. (2020). terraref/computing-pipeline: Season 4 & 6 Data Publication (2019).
- Burnette, M., ZongyangLi, Hajmohammadi, S., LeBauer, D., Heyek, N., and Willis, C. (2019f). terraref/extractors-3dscanner: Season 6 Data Publication (2019).
- Chamberlain, S., Foster, Z., Bartomeus, I., LeBauer, D., Black, C., and Harris, D. (2019). traits: Species Trait Data from Around the Web. R package version 0.4.2.
- LeBauer, D., Heyek, N., Shekar, R., Leinweber, K., Maloney, J., and Dornbusch, T. (2020a). terraref/reference-data: Season 4 & 6 Data Publication (2019).
- LeBauer, D., Willis, C., Shekar, R., Burnette, M., Li, T., Rohde, S., Liu, Y., Maloney, J., Fahlgren, N., Zender, C., Kooper, R., JeromeMao, harshagrawal28, Hong, X., Bradley, S., Pessé, S., Leinweber, K., Manzo, J., Terstriep, J., and Stylianou, A. (2020b). terraref/documentation: Season 6 Data Publication (2019).

BIBLIOGRAPHY 19

Mao, J., Burnette, M., Butowsky, H., Zender, C., LeBauer, D., and Paheding, S. (2019). terraref/extractors-hyperspectral: Season 6 Data Publication (2019).

- Marini, L., Kooper, R., Gutierrez, I., Sophocleous, C., Burnette, M., Nicholson, T., Ondrejcek, M., Zhang, B., Zharnitsky, I., Satheesan, S. P., Padhy, S., Zhao, Y., Liu, R., Vaidya, A., Myers, J., Felarca, M., Angelo, B., Roeder, G., Lee, J., Hennessy, W., Issaranon, T., Guo, Y., Yuan, X., Kethineedi, V., Kumar, A., Nayudu, N., Poelmans, W., Jansz, W., Jansen, G., Navarro, C., Pitcel, M., Tenczar, N., Wang, C., Lambert, M., and McHenry, K. (2019). Clowder: Open Source Data Management for Long Tail Data.
- Rohde, S., Crott, C., Mulroony, P., Kemball, J., LeBauer, D., Kooper, R., Chen, J., Shirk, A., Yang, Z., Burnette, M., Saraf, U., and Dietze, M. (2016). bety: Betydb 4.6.
- Selby, P., Abbeloos, R., Backlund, J. E., Basterrechea Salido, M., Bauchet, G., Benites-Alfaro, O. E., Birkett, C., Calaminos, V. C., Carceller, P., Cornut, G., Vasques Costa, B., Edwards, J. D., Finkers, R., Yanxin Gao, S., Ghaffar, M., Glaser, P., Guignon, V., Hok, P., Kilian, A., König, P., Lagare, J. E. B., Lange, M., Laporte, M.-A., Larmande, P., LeBauer, D. S., Lyon, D. A., Marshall, D. S., Matthews, D., Milne, I., Mistry, N., Morales, N., Mueller, L. A., Neveu, P., Papoutsoglou, E., Pearce, B., Perez-Masias, I., Pommier, C., Ramírez-González, R. H., Rathore, A., Raquel, A. M., Raubach, S., Rife, T., Robbins, K., Rouard, M., Sarma, C., Scholz, U., Sempéré, G., Shaw, P. D., Simon, R., Soldevilla, N., Stephen, G., Sun, Q., Tovar, C., Uszynski, G., Verouden, M., and consortium, T. B. (2019). BrAPI—an application programming interface for plant breeding applications. *Bioinformatics*, 35(20):4147–4155.
- Willis, C., LeBauer, D., Burnette, M., and Shekar, R. (2020). terraref/sensor-metadata: Season 4 & 6 Data Publication (2019).