A new CAM6 + DART reanalysis with surface forcing from CAM6 to other CESM models

Kevin Raeder1,4*, Timothy J. Hoar1,4, Mohamad El Gharamti1,4, Benjamin K. Johnson1,4, Nancy Collins1,4, Jeffrey L. Anderson1,5, Jeff Steward2,4 & Mick Coady3,5

An ensemble Kalman filter reanalysis has been archived in the Research Data Archive at the National Center for Atmospheric Research. It used a CAM6 configuration of the Community Earth System Model (CESM), several million observations per day, and the Data Assimilation Research Testbed (DART). The data saved from this global, ∼1° resolution, 80 member ensemble span 2011–2019. They include ensembles of: sub-daily, real world, atmospheric forcing for use by all of the nonatmospheric models of CESM; weekly, CAM6, restart file sets; 6 hourly, prior hindcast estimates of the assimilated observations; 6 hourly, land model, plant growth variables, and 6 hourly, ensemble mean, gridded, atmospheric analyses. This data can be used for hindcast studies and data assimilation using component models of CESM; CAM6, CLM5, CICE5, POP2, MOM6, MOSART, and CISM; and non-CESM Earth system models. This large dataset (~120 Tb) has a unique combination of a large ensemble, high frequency, and multiyear time span, which provides opportunities for robust statistical analysis and use as a machine learning training dataset.

“Data assimilation” ("DA") is the term used in many geophysical sciences for the merging of observations with a model state created by a (usually) numerical model of the physical system. The model state used in this dataset is a “hindcast” because it represents a past state1. The model state is referred to as "prior" to the assimilation. The result of assimilating observations into a hindcast is a "reanalysis", which is a better description of the system than either the observations or the model state individually. Observations and model hindcasts have both valuable information and errors. Successful DA keeps the information from both and reduces the errors. It also reduces the prior uncertainty2,3.

The reanalyses created by the Data Assimilation Research Testbed4,5 (DART) use an 80 member ensemble of similar hindcasts, which leverages the power of statistics to give a more comprehensive estimate than a single hindcast can provide. The ensemble of reanalyses is a sample of the probability distribution of the physical system after the observations are assimilated (the “posterior”)6.

The mean of this ensemble can be viewed as the most likely weather. The spread of the ensemble tells us how much confidence to have in it (smaller spread implies more certainty) or how much variability we should expect.

DA was developed to improve the initial conditions used in numerical weather forecasts1, but its use is spreading into studies of other Earth system components; the oceans, land, cryosphere, etc. These components are strongly forced by the atmosphere. In order to successfully model them, the atmospheric forcing must be specified correctly, both its mean and variability. The first motivation for the creation of this dataset was to provide that forcing in the context of an Earth system modeling framework, in which the atmospheric forcing can be applied to the nonatmospheric components consistently and conveniently. This is accomplished by running an atmospheric reanalysis for as long as possible and archiving all of the fluxes and other variables as frequently as required by the nonatmospheric models. Then the nonatmospheric models can be run repeatedly without the cost of regenerating the atmospheric forcing. The nonatmospheric model runs could be single or ensemble hindcasts to study the model behavior, or they could be the hindcasts used in generating reanalyses of the non-atmospheric components (see Fig. 1 for an illustration).

1National Center for Atmospheric Research, CISL/DAReS, Boulder, CO 80305, USA. 2Spire Global Inc., 1690 38th St, Boulder, CO 80301, USA. 3National Center for Atmospheric Research, CISL/CSG, Boulder, CO 80305, USA. 4These authors contributed equally: Kevin Raeder, Timothy J. Hoar, Mohamad El Gharamti, Benjamin K. Johnson, Nancy Collins and Jeff Steward. 5These authors jointly supervised this work: Jeffrey L. Anderson and Mick Coady. 6email: raeder@ucar.edu
Several studies have found that successful ensemble DA using non-atmospheric models requires an ensemble of atmospheric forcing in order to maintain appropriate ensemble spread among the non-atmospheric model states. There are other useful data products created as part of the atmospheric DA process. They are archived for future repeated use. These include data which reveal the quality of the reanalyses. The quality was monitored frequently during the assimilations by comparing the 6 h model hindcasts to the observations that were about to be assimilated into those states. This comparison is made by generating ensemble model estimates of the observations at the observation locations, then generating statistics of the differences from the actual observations. The statistics include the bias, RMSE, and “total spread”, a combination of the ensemble spread and observation error which is used to judge the size of the other statistics. These prior estimates of the observations were archived for further evaluation. They are non-gridded data, so, for convenience, the graphics generated for evaluation were also archived. Other data in this set can be used to start atmospheric hindcasts or data assimilation experiments, which have many uses, including model performance evaluation, studies of atmospheric phenomena, and even exploration of a variety of assimilation algorithms which are available in DART. The last major dataset can be used to evaluate how the land model (CLM5) translates realistic atmospheric forcing into plant growth. These are described in detail in the sections that follow.

This dataset is a unique combination of a large ensemble, a multi-year time span, high frequency, and a global model constrained by observations. Such a dataset is challenging to create and archive, in terms of both computer resources and personnel time, as well as requiring careful consideration of the model definition and DA tuning. We believe that making it freely available will accelerate research in the Earth sciences.

**Methods**

**Overview.** Workflow of ensemble data assimilation. This reanalysis dataset is the result of a 9 year long series of assimilation cycles. Each cycle (see Fig. 2) consists of a 6 h, ensemble hindcast calculated by a CAM6 configuration of CESM2.1 (respectively; Community Atmosphere Model v.6, Community Earth System Model v2.1) (details in “Hindcast model”). The resulting model states are passed to DART, which modifies them to be more consistent with the set of observations available at that time (details in “Observations” and Table 7). At the end of each month of cycling, the results are evaluated. If they pass inspections, they are repackaged into more convenient formats and archived. The algorithms employed by DART are described in “Assimilation software”. Selected results from the hindcasts and assimilation are saved for immediate or later use, as described in the rest of the paper.

Context for understanding the data products. Given the major anticipated uses of these products in CESM and DART contexts, the data organization and description are motivated by the files created and used by those packages, instead of by the individual fields which may interest some researchers. In fact, many files contain a large number of variables which only have meaning in the context of CESM or DART, so this Data Description will not describe those. They are intended to be used, but not evaluated out of context. It will describe other fields which may be interesting outside of their usefulness in those packages.

The millions of files created by the assimilation process have been thinned, condensed, and packaged into more convenient units of data to facilitate archiving, discovery of desired data, downloading, and use.

Since the data spans 9 years, it includes a wide range of actual atmospheric behavior ranging from regional fronts and storms to multyear, global patterns like El Niño. The various data products have frequencies ranging from hourly (surface forcing) to four times/day to capture the daily cycles (e.g. the ensemble mean and sets of observations) to weekly (e.g. ensembles of CESM restart files). There is enough data saved weekly that the discarded data could be recreated at reasonable expense, if needed.

![Diagram of data flow](image) Figure 1. Illustration of an ensemble of data atmosphere surface fluxes from this reanalysis (and other required data) being fed to CESM’s coupler, which passes it to the ocean model. POP uses that data as an upper boundary condition during the evolution of the ocean model state. The model states are passed to DART for assimilation of ocean observations.
Figure 2. An illustration of the major parts of this ensemble data assimilation system. The red arrows highlight the core of the assimilation cycle. Black arrows indicate other data motion. "RDA" is the Research Data Archive. A cycle starts with a 6 h, ensemble hindcast, which passes an ensemble of model states to DART. DART assimilates the available observations into this prior ensemble. The resulting modified, posterior, model states are used by the hindcast model as initial conditions for the next hindcast. A flowchart of “Observation Space Diagnostics” (lower left box) is shown in Fig. 6.

The high frequency, ensemble mean data sample the climatological distributions, while the ensemble adds information about the local model attractor structure, given the observational constraints (the model attractor is the climatology generated by the model when it is free to run without being constrained by observations). This combination of frequent mean and less frequent full ensemble describes both large-scale and small-scale characteristics of states related to the model attractor when it is constrained to be close to observations. This is a CMIP6 model configuration of CESM2. There exist other samples from this model’s climatological attractor, which were unconstrained by atmospheric observations, other than the tuning of parameterizations to maximize the performance as a climate model. For example, see "Multi Model Large Ensemble". This dataset can be compared to those to identify model biases and estimate the fidelity of the model in years long simulations.

Software environments. Almost all of the data products are in NetCDF-4 compatible format, so a wide variety of tools can be used to access and manipulate the data. However, DART and CESM are both software environments which have been developed to provide flexible and effective use of these products. They also include user support in the forms of online and embedded documentation, tutorials, and issue forums. Making use of these environments can accelerate research using these datasets.

The core programs of both packages are written in Fortran for efficiency, especially when running on supercomputers. Both packages are usually run in Unix environments (DART scripts are mostly csh). CESM scripting requires Python.

DART is designed to efficiently use MPI parallelism, but not threading (e.g. OpenMP), so CESM is configured to use the same parallelism. On NCAR's Cheyenne supercomputer we found it highly beneficial to set two MPI environment variables to larger values than the defaults. In CESM's env_mach_specific.xml:

```xml
<environment_variables>
  <env name="MPI_COMM_MAX">16383</env>
  <env name="MPI_GROUP_MAX">1024</env>
</environment_variables>
```

Assimilation components description. Observations. The observations and retrievals (quantities derived from raw observations) used to create this dataset were gathered from a variety of publicly available sources. These include wind and temperature observations from airplanes, radiosondes, and retrievals from satellite observations, and Global Positioning System (GPS) refractivity observations (basically density) from COSMIC satellites, for example.

The sources of the observations were:

- From NCEP’s PREPBUFR files (prepqm) in NCAR's Research Data Archive: (ds090.0):
  - radiosondes from balloons, mostly over land.
  - ACARS from commercial aircraft, mostly over North America.
  - AIRCRAFT from commercial aircraft.
  - CDW Cloud drift winds from GOES satellites.
From COSMIC: Global Positioning System satellites radio occultation. Importing them to DART is described in your_DART/observations/obs_converters/gps/gps.html.

From AIRS: Infrared soundings from the AQUA satellite (Aqua_AIRS_Level2, AIRS2RET.006). Importing them to DART is described in your_DART/observations/obs_converters/AIRS/AIRS.html. In addition, the observations were thinned by using only every ninth observation along track and every tenth observation cross track.

The list of observation types used by this reanalysis is in Table 7. The observation error of each observation was taken from the original data source, and is stored with the observation values in this archive. See “Observation sequence files” for details. In some cases the error specified is larger than it could be. This is discussed briefly in “Observation space diagnostics”. The only harm of this is that those observations will be underweighted in the assimilation process; other similar observations and the model will have stronger influences. There are several million observations per day. A subset of the observations from one assimilation time are shown in Fig. 3.

The observations are repackaged into binary files with a format that satisfies DART’s requirements. Conversion to ASCII is available, via a DART program, and interpretation of the contents is available in the DART documentation. See “Observation sequence files”.

**Hindcast model.** The released version of CESM2.1 used here contains models of all the parts of the Earth system that influence the weather: atmosphere, ocean, land, sea and land ice, biogeochemistry, etc. Communication between these components is controlled by the “coupler”. Each component can be “active” (calculating the evolution of the model state), “data” (reading a model state that was generated elsewhere), or “stub” (no data passed to or from that component). The mode of each component is defined by a “compset” (component model
This reanalysis used the compset HIST_CAM60_CLM50%BGC-CROP_CICE%PRES_DOCN%DOM_MOSART_SGLC_SWAV which is parsed as in Table 1. HIST does not describe a component. It means that initial conditions are historical (not from a climate projection).

CAM's "resolution" variable defines the horizontal grid and the dynamical core, which in this case is the Finite Volume core, which is defined on a logically rectangular grid with spacing \( \sim 0.9 \, ^\circ \) in latitude and \( 1.25 \, ^\circ \) in longitude. The land model (CLM5) uses the same grid. The vertical resolution is defined by the choice of the atmospheric component. For CAM6-FV it is 32, hybrid \( \sigma \) + pressure levels, which are terrain following ("\( \sigma \)" near the surface (the pressure on a level varies from place to place), constant pressure surfaces near the top, and a mixture of the two in the middle. The levels range from 7.44 hPa above the model ground up to a height of 3.64 hPa.

The data ocean model reads sea surface temperature (SST) and sea ice coverage data from files containing AVHRR data. The spatial resolution of this data is higher (\( 0.25 \, ^\circ \)) than CAM. The temporal resolution is nominally daily, but represents an ocean state which is a weighted average of data from several days. See "Sea surface temperature and ice coverage" for details.

Additional external forcing of CAM includes specified aerosols, greenhouse gases, and volcanic forcing, from CESM datasets. These are historical data for dates through 2014, and use CMIP6 scenarios after that. More information about these datasets is in "Files that force CAM".

Assimilation software. DART provides an extensive choice of algorithms for ensemble Kalman filter data assimilation\(^4\). Based on extensive experimentation, the choices in Table 2 define the assimilation algorithm which generated these reanalyses.

The model state is chosen to be the set of prognostic variables in CAM, which are required to define all other variables at the beginning of a hindcast. The models' states are stored in CAM "initial" files, from which both CAM and DART read them, and to which both write updated model states. See Table 6 for the list of variable names, which define the model state in a namelist in the input.nml file. Although the model state is defined using only atmospheric variables, and all observations are atmospheric, the land and sea ice variables evolve set, documented here).
consistently with the atmosphere, due to the coupling in the model. Those variables are passed along from cycle to cycle by being stored in those components’ “restart” files.

Note that there is no specification of the error covariances to use in the assimilation. The reason is that in the ensemble Kalman filter the background error covariance is never explicitly calculated. It is implicit in the algorithm, which calculates, at each time and for each observation, the correlation between the ensemble of model estimates of the observation and the ensemble of each model state variable. Large correlations result in large increments added to the state variable, and small correlations result in small increments.

Data management. The assimilation process generates a large amount of data in the form of large numbers of “small” files (Kbytes to several Gbytes), which are useful in the moment, but only some of which need to be archived. Those which need to be archived have been combined into files which have a convenient size for future use and make the data easier to find in the archive. In addition, they are compressed for efficient storage and transfer to where they are needed. This is described in “Data records”.

CESM model state at the start. The CESM compset used in this reanalysis has active components with a broad range of dynamical memory, due to differing levels of nonlinear behavior and inertia in the physical systems. The atmosphere has some long-lived constituents, which influence the weather, but their persistent influence is overwhelmed by the model’s perturbation error growth. Starting hindcasts with tiny differences in initial conditions and running them for 2 weeks results in model states that appear to be unrelated, other than being in the same season. There is also a relatively high density of atmospheric observations, so the model state can be brought into agreement with them in a time span measured in days. In contrast, the land model has large reservoirs of some constituents, which react slowly and non-chaotically to forcing from the atmosphere. There is a relatively low density of observations, especially below a few meters below the surface, so bringing an arbitrary land model state into agreement with observations can take months to decades of assimilation. This reanalysis dealt with those issues by starting an atmospheric assimilation 6 months before the reanalysis start date. This “spin up” assimilation used an ensemble of CLM model states, which itself had already been spun up for 12 years, forced by a “2 degree” CAM4 ensemble reanalysis.

Validation. We include a subsection about validation in “Methods” section because the results of our validation calculations are, themselves, one of the products in this dataset. They are available for further use, so the methods used to derive them should be described here. Further validation details are in “Technical Validation”.

One of the most important aspects of the assimilation to keep in mind is that it balances the uncertainty in the model, as represented by its ensemble spread, and the uncertainty in the observations, as represented by the observation error variance. This balance is a function of field, location, and time, due to the heterogeneous distribution of observations and the range of weather phenomena which the model must describe. If the uncertainty in the model becomes too small, the assimilation will reject observations that appear to be outliers, even though they are valid observations. This can allow the spread to become even smaller, and so on, until the model has diverged from the observations and ignores almost all of them, in which case the assimilation has failed. This is prevented by the ensemble spread “inflation” algorithm.

Observation space diagnostics. Assimilation health can be monitored by processing the assimilation output periodically to examine the fraction of observations used as a function of time, and the bias and RMSE relative to the observations. The latter are calculated by comparing the model mean estimates of the observations to the actual observations at the observation locations, i.e. in “observation space”. We do not use the posterior model state because it may be overfit to the observations, which would give an overly optimistic representation of the assimilation. The assimilation results are compared against each observation type separately, e.g. a figure may show a time series of the bias of the model estimates of temperature relative to the radiosonde temperatures that were assimilated, but not relative to the aircraft temperatures, which are taken at different locations and times and may have different biases. Details of the DART diagnostic software and how to do further validations are described in “Observation sequence files”.

These ideas are illustrated in Fig. 4, which is derived from the “spinup” assimilation, which ensured that the initial ensemble of the reanalysis represented a stable pattern, with no remnants of the arbitrary initial conditions. The figure displays a useful quantity we call “total spread”. Since both the hindcast and observations have uncertainty associated with them, it is helpful to view them as probability distributions, each with its own spread around its most likely value, those being the ensemble spread (σ\(_{\text{model}}\)) and the observation error standard deviation (σ\(_{\text{obs}}\)). Whether the two distributions are distinct or essentially indistinguishable depends on both spreads, as well as the difference between the means. The total spread is a combination of the two spreads, σ\(_{\text{total}}\) = \(\sqrt{\sigma_{\text{obs}}^2 + \sigma_{\text{model}}^2}\), which can be used as a measure of whether the RMSE is “large” or not. The model state can be arbitrarily accurate, given enough good observations, so the RMSE can be arbitrarily small. The total spread, however, is always at least as large as the observation error standard deviation, which is independent of the ensemble model state and the assimilation. So we expect the RMSE to be less than or equal to the total spread. In practice, the RMSE is often less than the total spread, which indicates that the observation error is larger than it needs to be.

In Fig. 4 the initial ensemble has a tiny spread, so the total spread is small. This causes the assimilation to ignore more than half of the observations because it considers them to be impossible outliers. Note that the RMSE of the initial ensemble is relatively large, even though the observations that are farthest from the ensemble have been excluded from the RMSE calculation because the observations were rejected. So the ensemble has very
To demonstrate the assimilation process, a time series of quantities is plotted in Fig. 4. This figure shows the root mean square error (RMSE) and total spread of the model estimates relative to the observations, along with the number of observations available and assimilated at each time step. The RMSE is a measure of the model's accuracy, showing how well the ensemble estimates match the observations. The total spread indicates the model's uncertainty about the true state.

Around day 5, the total spread increases, allowing the assimilation to incorporate more observations, which in turn reduces the RMSE. This suggests that the ensemble estimate is becoming more accurate. By day 10, the RMSE has fallen significantly, indicating that the ensemble state has high confidence in a correct estimate. The assimilation process is considered healthy when the RMSE is approximately equal to the total spread.

The state space of the assimilation includes months where the model and observations are in a stable state, but there are features that require investigation. These could be sudden increases in the number of observations, such as during a hurricane season, which can be verified by examining the assimilation output on the model grid. The impact of these features on the assimilation process and the quality of the observations is a topic for further research.

Community evaluation. This ensemble reanalysis is a valuable resource for researchers and students at all stages of their careers. It provides a platform for learning about the assimilation process, answering questions, and collaborating on research projects.
Data records

Archive location and access. The reanalysis dataset has been archived in the Research Data Archive ("ds345.0") at the National Center for Atmospheric Research (NCAR). It is freely available, but a simple registration is required. The following subsections describe the data products as they are organized in the RDA site, which is consistent with the organization of the CESM short term archive. There are subdirectories for various groups of archived files. In each group directory there are subdirectories for either the ensemble members or dates archived there. A key to the outline of the archive is:

  "RDA PRODUCT name" (files_group_name [a link]),

ensemble member or date subdirectories
data files

Where, in the following,

| INST | 0001 · · · 0080 |
| YYYY | 2011 · · · 2019 |
| MM  | 01 · · · 12    |
| DD  | 01 · · · 31    |
| SSSS | 00000, (occasionally 64800) |

The files in the subdirectories are described in the subsections below. Follow the files_group_name links.

“CESM Flux Coupler (cpl7) Files” (cpl)
cplINST

| INST | YYYY | MM | DD | SSSS | cpl files |
|------|------|----|----|-----|-----------|
| f.e21.FHIST_BGC.f09_025.CAM6assim.011.cpl_INST.hr2x.YYYY.nc.gz |
| f.e21.FHIST_BGC.f09_025.CAM6assim.011.cpl_INST.ha2x3h.YYYY.nc.gz |
| f.e21.FHIST_BGC.f09_025.CAM6assim.011.cpl_INST.ha2x1hi.YYYY.nc.gz |
| f.e21.FHIST_BGC.f09_025.CAM6assim.011.cpl_INST.ha2x1h.YYYY.nc.gz |
| f.e21.FHIST_BGC.f09_025.CAM6assim.011.cpl_INST.ha2x1d.YYYY.nc.gz |

“CESM Atmosphere (CAM6.0) Files” (atm)
atmYYYYMM

| YYYY | MM | atm files |
|------|----|-----------|
| f.e21.FHIST_BGC.f09_025.CAM6assim.011.cam_allinst.e.forecast.YYYY-MM.tar |

“External System Processing (DART) Files” (esp = DART)

espYYYYMM

| YYYY | MM | esp files |
|------|----|-----------|
| Diags_NTrS_YYYY-MM.tgz |
| f.e21.FHIST_BGC.f09_025.CAM6assim.011.cam_obs_seq_final.YYYY-MM.tgz |
| f.e21.FHIST_BGC.f09_025.CAM6assim.011.dart.e.cam_forecast_mean.YYYY-MM.tar |
| f.e21.FHIST_BGC.f09_025.CAM6assim.011.dart.e.cam_forecast_sd.YYYY-MM.tar |
| f.e21.FHIST_BGC.f09_025.CAM6assim.011.dart.e.cam_output_mean.YYYY-MM.tar |
| f.e21.FHIST_BGC.f09_025.CAM6assim.011.dart.e.cam_output_sd.YYYY-MM.tar |
| f.e21.FHIST_BGC.f09_025.CAM6assim.011.dart.rh.cam_forecast_priorinf_mean.YYYY-MM.tar |
| f.e21.FHIST_BGC.f09_025.CAM6assim.011.dart.rh.cam_forecast_priorinf_sd.YYYY-MM.tar |
| f.e21.FHIST_BGC.f09_025.CAM6assim.011.dart.rh.cam_output_priorinf_mean.YYYY-MM.tar |
| f.e21.FHIST_BGC.f09_025.CAM6assim.011.dart.rh.cam_output_priorinf_sd.YYYY-MM.tar |

“CESM Land Model (CLM5.0) Files” (lnd)
lndINST

| YYYY | lnd files |
|------|----------|
| f.e21.FHIST_BGC.f09_025.CAM6assim.011.clm2_INST.h0.YYYY.nc.gz |
| f.e21.FHIST_BGC.f09_025.CAM6assim.011.clm2_INST.h1.YYYY.nc.gz |

“CESM Restart Files including Initial Files” (rest)

restYYYYMM

| YYYY | rest files |
|------|------------|
| f.e21.FHIST_BGC.f09_025.CAM6assim.011.INST.alltypes.YYYY-MM-DD-00000.tar |
| f.e21.FHIST_BGC.f09_025.CAM6assim.011.infl_log.alltypes.YYYY-MM-DD-00000.tar |
File naming conventions. In each of those directories are files, whose names roughly follow the CESM file naming convention ('[ ]' = optional part):

```
CASENAME.model[INST].filetype[subtype].DATE.extension[compression]
```

Tar (tape archive) files contain files which also follow this convention. The parts of the file name can be interpreted using Table 3. An example is f.e21.FHIST_BGC.f09_025.CAM6assim.011.cam_allinst.e.forecast.2011-01-03-00000.tar. More examples are listed in the relevant subsections, below.

**Surface forcing files.** The physical system components of CESM influence each other via fluxes and component variables at the Earth’s surface. CESM’s coupler mediates this communication and can write those fluxes and variables to “history” files for later use. This reanalysis produced the five different coupler history files needed to run combinations of CESM components which require a data atmosphere (with a few, rarely used exceptions). These files are intended to be used only in this way, so we will not describe each variable in each file, but will focus on how to use them. The files are in NetCDF format and contain useful metadata, such as variable long names, so individual variables can easily be extracted and evaluated, but researchers should be careful to learn the exact nature and provenance of those variables. Metadata can be misleading.

The files are written at the end of each 6 h hindcast, but contain data with a variety of frequencies, as appropriate for each variable. At the end of each year they are concatenated into year long time series for convenient archiving and later direct use by CESM. They are also compressed for efficient archiving and copying to local computers. Table 4 describes the CESM coupler history files and which CESM components need which ones.

An example of a file name is f.e21.FHIST_BGC.f09_025.CAM6assim.011.cam_allinst.e.forecast.2011-01-03-00000.tar. More examples are listed in the relevant subsections, below.

**Table 3.** The parts of CESM file names, their interpretation, and illustrative examples. The many filetypes will be described in the file description subsections, below.

| Part       | Description                                                                 | Examples                                                                 |
|------------|-----------------------------------------------------------------------------|--------------------------------------------------------------------------|
| CASENAME   | CESM ‘CASENAME’                                                             | f.e21.FHIST_BGC.f09_025.CAM6assim.011                                   |
| model      | CESM component model                                                        | cpl, cam, clm,                                                          |
| INST       | The [optional] ensemble member(s)                                           | 00080, allinst ('instance' is the CESM name for ensemble member.)        |
| filetype   | Abbreviated type of file                                                    | 'i'ntial, 'e'xternal system processing, ha2x1d = 'h'istory 'a'tm to any '1'day frequency. |
| subtype    | Refinement of the filetype                                                  | 'f'orecast' file from filetype 'e'                                        |
| DATE       | Hindcast date and time label                                                | 2011-01-03-00000, 2019-12                                                |
| extension  | Abbreviation of the file format                                             | nc (NetCDF), tgz (gzipped tar file)                                      |
| compression| Abbreviation of the compression used                                        | gz (gzip)                                                                |

**Table 4.** Which forcing file filetypes are used by which CESM component models in “data atmosphere” mode. Depending on the compset chosen, these components may need forcing files from components in addition to the DATM. In that case, a case can be set up and run to use the DATM forcing files and write out the additional forcing.

| active component | Filetype →          | ha2x1d | ha2x3h | ha2x1h | ha2x1hi | hr2x1d |
|------------------|---------------------|--------|--------|--------|---------|--------|
| Ind: CLM, CTSM   | Yes                 | Yes    | Yes    | Yes    | Yes     |        |
| ocn: POP, MOM    | Yes                 | Yes    | Yes    | Yes    | Yes     |        |
| ice: CICE        | Yes                 | Yes    | Yes    | Yes    |         |        |
| gle: CISM        | Yes                 | Yes    | Yes    | Yes    |         |        |
| rof: RTM, MOSART | Yes                 | Yes    | Yes    | Yes    |         |        |

NOTE: CESM generally interpolates these data to the start time requested by the user. In order to start a hindcast on the first date of the dataset (2011-01-01-00000), the 2011 forcing files must contain data from the end of 2010. This sometimes raises questions about whether the “time” variable, and “time:units” and “time:bounds” metadata are all correct. They are.
Restart file sets. CESM is able to fully stop and restart with results that are identical to a case where it doesn't stop. It does this by writing and reading comprehensive “restart” files, which contain a complete description of the state of the model. In the context of ensemble assimilation, it writes a restart file set for each ensemble member. A restart set for one member (INST) for one date is stored in the RDA in a file like `f.e21.FHIST_BGC.f09_025.CAM6assim.011.INST.alltypes.YYYY-MM-DD-00000.tar` where “alltypes” indicates that a variety of filetypes are contained in it. See the CESM file naming conventions for details about these standard filetypes. The list of files in such a file can be found in Table 5. The variables in some of the files will be described in sub-sections, below.

These restart sets can be used to start single or ensemble hindcasts, and to start data assimilation experiments. Each ensemble member is an equally likely model state, so they can be chosen at random, unless a specific atmospheric feature is needed, such as the strongest hurricane in the ensemble. They are available every Monday at 00:00 UTC.

CAM initial files. In this reanalysis CAM6 is instructed to write out an ensemble of “initial” files at the end of each hindcast. See Table 5 for an example file name. They contain the variables which comprise the DART prior state vector, and enough other variables to start a CAM6 hindcast (Table 6). In contrast to the “restart” files, they cannot resume a previous hindcast in a continuous manner. Initial files were chosen over restart files for the storage of the state variables for several reasons:

- smaller size (less than 1/3),
- more intuitive variables (e.g. sensible temperature instead of scaled virtual potential temperature),
- better metadata,
- no need for identical hindcast continuation.

That last reason is because DART changes the model state variables between the end of the previous hindcast and the start of the next, so identical continuation is not possible.

Table 5. The list of files in a “restart set”, their filetypes, and example file names (CASENAME = f.e21.FHIST_BGC.f09_025.CAM6assim.011). The history files are not required for an exact restart of the model, but are archived with the restart files to maintain continuity of optional time series of (time averaged) fields requested from the case. The relationship between history and restart history files is described in CESM Post Processing Data. The DART inflation restart history files are not used during CESM's restart process, but are used by the assimilation. They are also archived more frequently with the other DART output as described in “Ensemble mean and spread files”.

| Component model | File type     | File name                                           |
|-----------------|---------------|-----------------------------------------------------|
| CAM6            | Initial       | CASENAME.cam_0080.i.2020-01-01-00000.nc            |
| CAM6            | Restart       | CASENAME.cam_0080.r.2020-01-01-00000.nc            |
| CAM             | Surface restart | CASENAME.cam_0080.rs.2020-01-01-00000.nc        |
| CICE            | Restart       | CASENAME.cice_0080.r.2020-01-01-00000.nc          |
| CLM5            | Restart       | CASENAME.clm2_0080.r.2020-01-01-00000.nc          |
| cpl7            | Restart       | CASENAME.cpl_0080.r.2020-01-01-00000.nc           |
| MOSART          | Binary restart | CASENAME.mosart_0080.r.2020-01-01-00000          |
| DCCN            | Binary restart | CASENAME.docn_0080.rs1.2020-01-01-00000.bin   |
| CAM             | History #0    | CASENAME.cam_0080.h0.2019-12-31-64800.nc         |
| CLM             | History #0    | CASENAME.clm2_0080.h0.2020-01-01-00000.nc        |
| CLM             | History #1    | CASENAME.clm2_0080.h1.2020-01-01-00000.nc        |
| MOSART          | History       | CASENAME.mosart_0080.h0.2020-00-nc               |
| CLM             | Restart history #0 | CASENAME.clm2_0080.rh0.2020-01-01-00000.nc    |
| CLM             | Restart history #1 | CASENAME.clm2_0080.rh1.2020-01-01-00000.nc    |
| MOSART          | Restart history #0 | CASENAME.mosart_0080.rh0.2020-01-01-00000.nc |
| DART            | Restart history | CASENAME.dart.rh.cam_forecast_priorinf_mean.2020-00.nc |
| DART            | Restart history | CASENAME.dart.rh.cam_forecast_priorinf_sd.2020-00.nc |
For the curious, here is an overview of the file contents. The CAM restart files contain similar variables to the initial files, but many more (184 versus 36). There is no metadata for many of them and some do not even appear in the CAM log file “MASTER LIST.” The CLM restart files have 276 variables, whose metadata includes their long names, and 143 more which lack that. The coupler restart files contain 203 variables, many of which are related to the variables in the coupler history (“forcing”) files. They contain additional fluxes from non-atmospheric (or river) components, such as CICE and CLM. The CICE restart files contain 54 variables with no metadata. Consult the User’s Guide if needed. The river runoff (MOSART) restart files contain 14 variables on a longitude–latitude grid, with long name metadata.

Inflation files. Following Bayes’ theorem, the prior distribution (represented by an ensemble) is combined with the observations at each assimilation cycle to produce a posterior. If the spread of the prior is small due to model and sampling errors or if the observation estimate is overconfident, the posterior will also be overconfident. This is easy to view because after applying Bayes’ rule, the posterior variance will be smaller than both the prior and observation error variances. The easiest way to fix that is to “inflate” the ensemble; increase the spread of the ensemble around its mean, while preserving the mean. In large, complex models such as CAM6, an effective algorithm for doing that is adaptive inflation, which defines an inflation value (and standard deviation) at each model grid point for each state variable, and evolves them in time in order to adapt to the evolving distribution of observations and model state. The inflation can be applied to the prior or posterior ensemble. Studies have shown that prior inflation can mitigate model biases while posterior inflation is effective at reducing sampling errors. Model biases often dominate sampling errors. In this reanalysis study, we use the adaptive prior inflation algorithm described in El Gharamti et al.

This evolving inflation data is stored in “inflation restart files” during each assimilation cycle. The product of the algorithm is essentially a distribution, so the inflation is written out as a pair of mean and standard deviation inflation files. These files describe the state of the inflation algorithm. Examples of those file names are in Table 6.

### Table 6. The CAM6 variables which are written to the initial files. The state variables are those that are directly changed by the assimilation. The rest evolve in response to the changes to the state variables as well as the model physics and dynamics. The “modes” in the MAM4 modal aerosol scheme are “accum” (1), “aikten” (2), “coarse” (3), and “primary_carbon” (4).

| Variable name | Description |
|---------------|-------------|
| PS            | Surface pressure |
| T             | Sensible temperature |
| US            | Zonal wind component (on a grid staggered latitudinally 1/2 grid box) |
| VS            | Meridional wind component (on a grid staggered longitudinally 1/2 grid box) |
| Q             | Specific humidity |
| CLDLIQ        | Cloud liquid water (grid box average) |
| CLDICE        | Cloud ice (grid box average) |
| NUMICE        | Cloud ice number (grid box average) |
| NUMLIQ        | Cloud liquid number (grid box average) |
| NUMRAI        | Rain number (grid box average) |
| NUMSNOW       | Snow number (grid box average) |
| RAINQNM       | Rain amount (grid box average) |
| SNOWQNM       | Snow amount (grid box average) |
| Aerosols      | Dimethyl sulfide |
| DMS           | H2O2 |
| H2SO4         | SO2 |
| SOAG          | Secondary organic aerosols gas |
| bc_a[1,4]     | Black carbon, modes 1 and 4 |
| dst_a[1–3]    | Dust, modes 1 through 3 |
| ncl_a[1–3]    | Sea salt (NaCl), modes 1 through 3 |
| num_a[1–4]    | Aerosol number density, modes 1 through 4 |
| pom_a[1,4]    | Primary-organic aerosols, modes 1 and 4 |
| soa_a[1,2]    | Secondary-organic aerosols, modes 1 and 2 |
| so4_a[1–3]    | Sulfate (SO4, modes 1 through 3 |

The CAM6 + DART model state variables

The other moisture variables

Other aerosols

MAM4 modal aerosol scheme variables

For the curious, here is an overview of the file contents. The CAM restart files contain similar variables to the initial files, but many more (184 versus 36). There is no metadata for many of them and some do not even appear in the CAM log file “MASTER LIST”. The CLM restart files have 276 variables, whose metadata includes their long names, and 143 more which lack that. The coupler restart files contain 203 variables, many of which are related to the variables in the coupler history (“forcing”) files. They contain additional fluxes from non-atmospheric (or river) components, such as CICE and CLM. The CICE restart files contain 54 variables with no metadata for them. Consult the User’s Guide if needed. The river runoff (MOSART) restart files contain 14 variables on a longitude–latitude grid, with long name metadata.
Figure 5. The mean values of the adaptive inflation coefficients for the zonal wind component (US) on the \(\approx 200\) hPa (top) and \(\approx 860\) hPa (bottom) model levels on Sep. 1, 2016 at 00 UTC. The inflation mean is defined for all model state variables at all assimilation times. It is a dimensionless quantity. Note the relationship between the inflation values at 200 hPa and the density of ACARS temperature observations shown in Fig. 3c. Similarly for the 860 hPa inflation values and the radiosonde US observations in Fig. 3a. The inflation standard deviation is constant (0.6) everywhere for all model state variables, so it is not shown. The figure, including continental outlines, was drawn using ncview (version 2.1.7), which is open source software licensed under the Gnu General Public License version 3.

Table 7. The names of the observation types available in the obs_seq_final files can be constructed by combining an entry from the first column (e.g. AIRS_) with an entry from the top row (e.g. TEMPERATURE), e.g. AIRS_TEMPERATURE. That type is the name for retrievals of temperature from the AIRS instrument on the AQUA satellite. QTY is an abbreviation for DART's "quantity", which denotes what is being measured, while TYPE denotes the source of the measurement. Each type was either assimilated, evaluated, (blank) ignored, or 'X' doesn't exist.
the restart file Table 5 and have the filetypes rh.cam_forecast_priorinf_mean and rh.cam_forecast_priorinf_sd. These files have variables named the same as the model state variables (see Table 6), but their contents are inflation values, defined by the filetype. The inflation fields are useful for evaluating the assimilation performance, and they are relatively small, so they are archived for every cycle. The subset of these files, which are archived as part of the restart file sets, are in archive files having "infl_log" in their names, e.g. as in the restart files outline. See Fig. 5 for examples of the inflation mean fields.

**Atmosphere model ensembles.** The whole ensemble of prior model states is archived at least weekly in files of the form fc21.FHIST_BGC.f09_025.CAM6assim.011.cam_allinst.e.forecast.YYYY-MM-DD-SSSSS.tar (not to be confused with the "alltypes" files in restart sets). The posterior versions of the contents of these files are archived in the CAM initial files in the (weekly) restart sets (see Table 5) [NOTE: When the initial files were written they contained the prior model states (see "CAM Initial Files"). After the assimilation they contain the posteriors]. The assimilation innovations can be calculated by subtracting a prior (forecast) variable from its posterior (initial file) version, e.g. for temperature: $T_{\text{innovation}} = T_{\text{init}} - T_{\text{forecast}}$.

NOTE: Similar ensemble files with filetype "preassim" contain the inflated ensemble, which cannot be used to calculate assimilation innovation without deflating the ensemble first, using the inflation values described in "Inflation time series". This is in contrast to the innovations of the mean, which can be calculated from the ensemble mean of either "forecast" or "preassim". See "Ensemble mean and spread files".

**Assimilation files.** The program "filter", which does the assimilation, writes out a variety of files, which were used to evaluate the health of the assimilation, but can also be a source of research data. They are described in detail in the following subsections.

**Observation sequence files.** DART currently requires that the observations to be assimilated and the metadata describing them be packaged into a custom formatted file. The assimilation process generates an ensemble of model estimates of each observation, which are written, with the actual observations, to an "obs_seq_final" file using the same custom format. In this reanalysis the files are binary for compactness.

At the end of each month of assimilation the obs_seq_final files are compressed into a tar archive for archiving in the RDA. The file names have the form fc21.FHIST_BGC.f09_025.CAM6assim.011.cam_obs_seq_final.YYYY-MM.tar

The observation types, which were assimilated (e.g. RADIOSONDE_TEMPERATURE), are a subset of the types available in the obs_seq_final files. Other types were merely "evaluated" during the assimilation, meaning that filter calculated the ensemble model estimates of the observations, but did not change the model state to fit them better. These are often referred to as "withheld" observations, which provide an independent verification of the assimilation. Table 7 lists the observation types and how they were used.

**Statistical representations of observation space performance.** In order to calculate the statistics of the observation data in the obs_seq_final files, as discussed in "Observation space diagnostics", program "obs_diag" harvests data from them, performs some of the statistical analysis, and writes the results into a NetCDF file ("obs_diag_output.nc"). This workflow, and related workflows, are outlined in Fig. 6. Obs_diag enables users to focus the evaluation in many ways. The following features of the evaluation can be specified as inputs to obs_diag:

- observation types
- horizontal and vertical domains
- date range of the data
- statistics or variables displayed (bias, RMSE, total spread, rank histograms, and more)

DART provides Matlab© scripts to read the obs_diag_output.nc files, finish the statistical analysis, and display the results. (see "Assimilation diagnostic files" for guidance about replacing the Matlab© scripts by similar software of the user's choosing.) The resulting files are packaged into files of the form "Diags_NTrS_YYYY-MM.tgz", which contain the following files, most of which are described by a template due to the large number of similar names. Not all combinations of TYPE and QTY could be generated; see Table 7 for a map.

```
obs_diag_output.nc (statistics generated by program obs_diag)
  script.m (Matlab© script which created the .ps and .pdf files)
  matlab_nc.out (diagnostic output from script.m)
  TYPE_QTY_rmse_bias_evolution_region#.ps
  TYPE_QTY_rmse_totalspread_evolution_region#.ps
  TYPE_QTY_rmse_bias_profile_region#.pdf
  TYPE_QTY_rmse_bias_norm_profile_region#.pdf
  TYPE_QTY_rmse_totalspread_profile_region#.pdf
  TYPE_QTY_rmse_bias_obscount.txt
```

Where

YYYY = 2011 . . 2019
MM = 01 . . 12.
Figure 6. A map of the observation space diagnostics software available in DART. The CAM6+DART cycling (Fig. 2) creates a time series of binary obs_seq_final files, which have a custom format. They are easily converted to NetCDF using DART’s obs_diag.f90 and obs_seq_to_netcdf.f90 programs. The obs_diag_output.nc file has the time series concatenated into it. The obs_epoch_#.nc files map one-to-one to the obs_seq_final files, and are numbered sequentially. Then a wealth of statistics (Table 8) can be calculated and displayed by DART’s suite of Matlab scripts (.m). The resulting .pdf and .ps pictures are suitable for presentations.

An illustration of time series from this type of analysis is in Fig. 4 and is discussed in “Observation space diagnostics”. A more condensed view of some of the data in this reanalysis is shown in Fig. 7. This picture provides examples of many features of the assimilation and evaluation, which are helpful for understanding the data products. The statistics shown there are calculated at the observation locations, so any interpolation is performed on the model state, not on the observations. The vertical dimension is divided into 14 layers, each of which contains a standard or mandatory pressure level of the atmosphere. The layers are not the model vertical levels. The figure also shows the number of observations available and the number assimilated in each layer, which provide guidance about the health of the assimilation (a large fraction assimilated is healthy) and about the trustworthiness of the RMSE and bias (small number assimilated = untrustworthy). Note that there are no observations assimilated in the top two layers, due to a choice to avoid assimilation in the top levels of the model, which are damped and don’t respond well to assimilation.

The observations in Fig. 7 come from low orbit satellites, such as COSMIC, which very accurately measure the transit time of radio signals emitted by Global Positioning System satellites. The times are distorted by the atmosphere, which makes it possible to calculate the atmospheric index of refraction. The index is reported as the observation, but is more accurately called a “retrieval” because it is derived from the raw measurements. Note that, despite the fact that the retrievals are not model state variables, they can be assimilated and provide information which is useful for updating the model state variables. The actual index values are near 1.0, but the reported numbers have the form \( n_{rep} = (n_{whole} - 1.0) \times 100 \) in order to focus on the variable part of the numbers. The index of refraction is a function of atmospheric density, which decreases exponentially with height. The profiles have been normalized by the average \( n_{rep} \) in each layer, so that the curves in the upper layers don’t appear to be “zero”. During this month in this region, all of the biases happen to be \( \geq 0 \), which reveals that CAM6 has...
a denser atmosphere than the observations indicate. Further probing reveals that a cold bias explains some of this density bias (not shown). This reanalysis reveals a variety of persistent biases in the model and/or in some of the observation platforms. The RMSE and bias shown in Fig. 7 are two examples of the quantities available in the obs_diag_output.nc files for visualization. The complete list of these “copies” is shown in Table 8, and is taken from the variable CopyMetaData in those files.

Some of the temperature bias mentioned in the discussion of Fig. 7 can be seen in Fig. 8, which shows pictures from the Diags_NTrS_2019-07.tgz file. In contrast to Fig. 4, these time series show an assimilation that has settled into a stable, healthy pattern. There is no obvious trend in any of the statistics, including the fraction of observations used. The fraction of RADIOSONDE_TEMPERATURE observations used is quite small in the layer displayed here because this reanalysis did not assimilate any observations below the bottom model level, which is ~ 52 m above the surface, and the surface itself is smoothed to be suitable for the model’s 1° resolution. The fraction used is much higher in higher layers and for other observations, such as AIRS (bottom of Fig. 8). A few of the time slots show relatively large (or small) RMSE and bias, which is almost always due to there being very few observations at that time, which can result in randomly bad (or good) agreement with the observations.

Since the bias of the model relative to both observation types is consistently ~ − 1 K, it is fair to conclude that the model probably has a deficiency. This bias persists despite the assimilation frequently pushing the model state towards the observations, so the bias in a free running hindcast would be larger. We should keep in mind the other possibility, that both observation platforms may be biased compared to reality and that the model is closer to the truth than both observation types, but we can’t confirm that from anything in this assimilation. The RMSE represents a combination of the bias and random error. A large portion of this RMSE is due to this bias, implying that the distribution of estimated observations is relatively narrow, which in turn implies that the model estimates are truly inconsistent with the observations and not just “different within the noise”. These

Figure 7. Profiles of the RMSE (black curve) and bias (green curve) of the ensemble mean estimates of the GPS refractivity retrievals (dimensionless) relative to the observed values, which were assimilated in the “Southern Hemisphere” (20°–90°S). The profiles have been normalized by the average in each layer. These profiles show the statistics of just the prior (“pr”) model states. The left axis numbers show the height (meters above the surface) of the standard or mandatory pressure levels (assuming a US standard atmosphere). All of the observations in a gray or white band have been binned together for analysis. The “grand” statistics (upper left corner) pool the observations from all layers. The red circles and plusses mark the number of observations available and assimilated in each layer (top axis). The (normalized) RMSE is dimensionless.
| Variable     | Description                                                                 | Use(s)                                                                 |
|--------------|------------------------------------------------------------------------------|------------------------------------------------------------------------|
| Nposs        | Number of observations available                                             | Helps assess the assimilation health                                   |
| Nused        | Number of observations assimilated                                           | Helps assess the assimilation health                                   |
| NbadQC       | Number of obs rejected due to flag from observation provider                |                                                                        |
| NbadDZ       | Number of excessive innovation Z scores                                      |                                                                        |
| NbadUV       | Number of unmatched U/V wind pairs                                          |                                                                        |
| NbadLV       | Number of obs excluded above the top, below the bottom                      |                                                                        |
| rmse         | Root mean square error                                                       | Shows the noisiness of the difference of the ensemble mean estimates   |
| bias         | Average difference of the mean estimates from the observations              | Reveals model and/or observation type biases                            |
| spread       | Combined spreads from ensemble estimates of all observations               | Focus on ensembles, or remove from total spread to see observation error|
| totalspread  | Combined ensemble spread and observation error of all observations          | Provides context for RMSE, bias, and assimilation health                |
| NbadDARTQC   | Number of observations not assimilated due to DART criteria                | Total observations that failed DART's quality control checks           |
| observation  | Average value of the actual observations in the region + time span          | Compare against the ensemble mean                                      |
| ens_mean     | Average value of the ensemble mean estimates of the observations            |                                                                        |
| N_trusted    | Number of observations designated as ’trusted’                              | These will be assimilated regardless of how different they are from the |
| N_DARTqc_0   | Number of observations given DART QC 0                                     | This number were assimilated                                            |
| N_DARTqc_1   | Number given DART QC 1                                                      | Only evaluated, not assimilated, following namelist instructions       |
| N_DARTqc_2   | Number given DART QC 2                                                      | Posterior forward operator failed after prior QC = 1                   |
| N_DARTqc_3   | Number given DART QC 3                                                      | Posterior forward operator failed after prior QC = 4                   |
| N_DARTqc_4   | Number given DART QC 4                                                      | Model estimates of observations could not be calculated                |
| N_DARTqc_5   | Number given DART QC 5                                                      | DART’s namelists prevented assimilation                                |
| N_DARTqc_6   | Number given DART QC 6                                                      | Prior forward operator failed                                          |
| N_DARTqc_7   | Number given DART QC 7                                                      | Observations were too far from the ensemble means                      |
| N_DARTqc_8   | Number given DART QC 8                                                      | DART failed to convert the observations’ vertical coordinates          |

Table 8. Obs_diag_output.nc files contain variables with a dimension (“copy”), which organizes the statistics of the contents of the observation sequence files (obs_seq_final). They are ordered in that file according to the CopyMetaData variable. Bold text highlights statistics which are displayed in the Diags_NTrS_YYYY-MM.tgz files. Further details can be found in the DART software package; .../your_DART/assimilation_code/programs/obs_diag/threed_sphere/obs_diag.html.

Biases are of the prior model states, which are in the atmospheric “Surface Forcing Files”. In contrast, the CAM initial files in the “Restart File Sets” contain posterior fields, which will generally have smaller biases because the assimilation has pushed those model states closer to the observations.

**Ensemble mean and spread files.** Filter also calculates the ensemble mean and spread in state space (on the model grid) and writes those to NetCDF files. Those files are written at two “stages”; the “forecast” and “output”, which are the “prior” and “posterior” states of the ensemble, respectively. Those features are summarized in the file type part of the file name, e.g. “output_sd” means the standard deviation (spread) of the output ensemble. They are available every 6 h. The impact of the assimilation on the model state ensemble mean can be calculated as “innovation = output - forecast”. Note that the “output” files have filetype “.i.” to signal that their contents describe the files which will be used to initialize the next hindcast, while the “forecast” files have filetype “.e.” to signal that they describe model data which will be modified by DART. All of these files contain only quantities describing the model state variables, (see the list in Table 6).

**Inflation time series.** The dart.rh files are concatenations of the inflation restart files, which are described in “Inflation Files” (p11), so they are 6-hourly time series. The rh.cam_output_priorinf* filetypes contain the same types of data as the rh.cam_forecast_priorinf*, but the fields have been updated by the assimilation. They were used by the subsequent assimilation.

**Land model time series.** The CLM namelists instructed it to write out “history” files of fields describing the evolution of plant growth under the influence of an ensemble of realistic atmospheric forcing. The fields were written to two files to separate the time averaging applied to each. Filetype “.h1” has time averaged values. Filetype “.h0” has instantaneous values. Files were written at the end of each 6 h hindcast, then concatenated into year long time series, and compressed for archiving. The requested fields, along with fields written by default, are listed in Table 9.
Files that force CAM. The component set chosen for this reanalysis uses a "data ocean" as a time evolving boundary condition which forces CAM6. While that dataset completely specifies the influence of the oceans on CAM, other datasets supply partial influences. These are added to related, internally generated fields, which are read from the initial files. One example is aerosols, which evolve according to model physics and chemistry, but also have contributions from sources outside of the atmosphere, such as industrial emissions. The files which provide this "external forcing" are provided in a CESM archive. Installation of CESM on most supercomputers includes at least parts of this archive in a location which is accessible to everyone. If these files are not in that archive, request that they be downloaded from the CESM data repository, which can be accessed by following instructions in the CESM User’s Guide. The namelist variables which specify the needed files are describe in the CESM2 CAM6 namelist variables page.

Figure 8. Time series of quantities derived from this reanalysis related to two observation platforms, as discussed in "Statistical representations of observation space performance". The red circles and asterisks mark the number of observations available and assimilated (right axis) at each time (bottom axis). The black dots and line show the root mean square error of the model ensemble mean estimates of the temperature (K) relative to the observed temperatures (left axis). The green squares and line show the bias (model ensemble mean-observation). The lines in the RADIOSONDE_TEMPERATURE picture are intermittent because times with no data are not plotted. In the region shown there are often no radiosonde observations at 06:00 and 18:00 UTC. These quantities were derived from a subdomain of the model; south of 20° S and from the surface to ~ 965 hPa high. The numbers in the legend labeled with “grand” are statistics of the entire month of data. The fraction and percentage in the title represent the fraction of observations used.
Sea surface temperature and ice coverage. The data which CESM reads to provide SSTs and sea ice coverage (but not thickness) was taken from the RDA dataset (ds277.7) before 2020, when it was replaced by files which have data valid at 12:00 UTC instead of 0:00 UTC. The 0:00 UTC data used in this reanalysis are archived in the RDA ds345.018 dataset avhrr-only-v2.2011-202001_0Z_filled_c200810.nc.gz.

Aerosols and greenhouse gases. For this CESM component set and for years before 2015 CESM chooses default files which contain historical data. For hindcasts in 2015 and later, there is a choice of using data in a “CYCLICAL” mode, which uses a specified year of data, or using CMIP6 scenario projections and the “INTERP_MISSING_MONTHS” mode. The scenarios are very similar during the first few years after 2014, so the choice is not of central importance. We chose files containing data from scenario “SSP3-7.0”, which specifies a moderate increase in greenhouse gas. The non-default files used in this reanalysis are listed in Table 10.

Land model. The CLM5 component of this reanalysis employed two external forcing files. Population density was read from firedata/clmforc.Li_2018_SSP3_CMIP6_hdm_0.5x0.5_AVHRR_simyr1850-2100_c181205.nc in SERIAL mode. Land use was read in CYCLICAL mode (year 2015 data) from file landuse.timeseries_0.9x1.25_SSP5-8.5_78pfts_CMIP6_simyr1850-2100_c181209.nc.

Log files. Further details about the hindcast model are in the weekly “infl_log” files. These include log files from the overall job (“cesm”), one of the 80 couplers (“cpl_0001”), and one each of the 5 nonstub components; cpl_0001, ice_0001, lnd_0001, ocn_0001, rof_0001. Log files from the assimilations are not archived in the RDA collection, but are available on NCAR’s Campaign Storage file system for a limited time. The most important aspects of the assimilation setup and results are described here and in the RDA dataset.

Technical validation
The intent of this project is to provide a useful representation of Earth’s actual weather for use in Earth system research, especially ensemble data assimilation. It is not to provide the best atmospheric reanalyses possible. As in any reanalysis, the fidelity to the weather depends on the types and numbers of observations at the time and in the area of interest, as well as on the ability of the model to simulate the atmospheric state. The validity of the data is described by some of the dataset itself, as noted in the “Validation” section. DART also provides methods for further evaluating these data products when a more focused evaluation is needed. See “Observation space diagnostics”, “Statistical representations of observation space performance”, and “Ensemble mean and spread
files” for examples and discussion. The suitability of this data for an application should be carefully evaluated independently of the evaluations available in this dataset. There is likely enough diagnostic data in this dataset that you can compare these results to reanalyses produced by operational centers.

**Monthly observation space evaluation.** Much of the technical evaluation of this reanalysis is contained in the monthly, observation space pictures generated by DART’s Matlab® scripts. That process is described in “Methods” and “Statistical representations of observation space performance”.

In addition to examining individual months, we compared the same month from all years to evaluate long term trends in the assimilation quality. Examples are shown in Fig. 9, which are not included in the reanalysis archive (e.g. Diags_NTrS_YYYY-MM.tgz) but could be recreated from the available data. Note that in Fig. 9a there is a dramatic decrease in the RMSE in layers 525 hPa and 400 hPa during the last 4 years and an increase in the number of observations assimilated. We believe that that is due to an improvement in 2016 in the algorithm used to calculate the wind from the movement of clouds. The RMSE values in the 100 hPa layer should be ignored because there were hardly any observations there, so the statistics are not robust.

Figure 9b shows generally larger temperature biases relative to radiosonde observations in the lower layers in recent years. We have not found an explanation for this trend, but have not seen any evidence that the reanalysis is failing. This sort of behavior could be the subject of further research.

**Ensemble spread.** The observation space diagnostics discussed in the previous sections show the fidelity of the model state ensemble mean to the observations. They basically answer the question “Is the model’s most likely estimate of the weather consistent with the observations?” An equally important question is “Is the consistency due to chance or to high certainty in the model ensemble?” That question is answered by the prior ensemble spread, which varies widely with location, time, and the atmospheric field of interest. An example is shown in Fig. 10. There is some correlation between the weather (ensemble mean, bottom figure) and the ensemble spread (top figure) in areas which are not well observed, such as the southern oceans. Well observed areas, such as over continents and down wind from them, have very small ensemble spread, indicating high confidence in the means.

**Use of the surface forcing files in CESM.** Multiple tests have demonstrated that the coupler history files (“forcing files”) can be read by CESM and provide atmospheric forcing for data atmosphere configurations of CESM (“DATM”), such as compsets whose short names start with “I” (CLM), “C” or “G” (POP2), and “D” or “G” (CICE). See Table 4 from “Surface Forcing Files”, Fig. 1, and the CESM compset web page for details.

**Reproducibility.** A reanalysis such as this is a complex activity, involving many layers of software, evolving computing environments, and human intervention. Fortunately, the core activity is comparison of model output
against observations, so the end product is closely tied to reality and is verifiable. Our intent in providing this dataset to the community is to prevent the needless reproduction of such a large amount of data. However, some reproducibility exercises are valuable for verification of the data products, the software used to create them, and how well data users understand it all. There are at least two varieties of reproducibility that are desirable from the various subsets of data; bitwise or statistical. Although the hindcast model and DART are designed to be capable of bitwise reproducibility, the fundamental nature and goal of ensemble data assimilation is a statistical description of the physical system. Two assimilations which use fundamentally the same hindcast model and the same assimilation algorithm, but different initial ensembles, should generate ensembles which are statistically indistinguishable after the typical spinup period. Conclusions drawn from such ensembles are robust and meaningful, while conclusions based on individual members or details of the differences between the the ensembles are generally not robust and are suspect.

**Bitwise.** The extent to which the results are bitwise reproducible will depend on many factors, including availability of the same or equivalent hardware, compilers, and libraries. The farther removed in time the reproduction effort is, the less likely it is to succeed, and the more effort it will take. For example, at one point some desirable output was lost during the archiving process. We attempted to recreate the data, after a significant computer upgrade, by recompiling the programs with the updated compilers to ensure consistency with the updated environment. We were unable to bitwise reproduce the data in the available time, but we discovered that the original executables, compiled before the upgrade, still reproduced earlier results exactly.

**Statistical.** When attempting to reproduce this reanalysis it is necessary to define an acceptable disagreement between the reproduction and the original. There is a range of standards which could be used, depending on the intended use. Some examples are, in roughly increasing precision:

Are the differences between the means smaller than the model state changes between assimilation times?
...smaller than the combined uncertainties of the two distributions?
...smaller than the assimilation innovations?

---

**Figure 9.** (a) The vertical profiles of the RMSE (ms⁻¹) of the zonal wind component of the prior model ensemble relative to the zonal, satellite, cloud drift, wind observations in December of each of 9 years (plus the spin-up year of 2010). It also shows the number of observations available (○) and used (⋆) during each December. Colors of all symbols are labeled in the legend. The “grand rmse” number is the RMSE relative to all of the observations in the month (i.e. all levels combined). (b) Same as ‘(a)’, but for the bias relative to radiosonde temperature observations (K⁻¹) in July.
Are the distributions indistinguishable using formal statistical methods of comparison, which take into account the possibility that the distributions are not random draws from the continuous distribution which represents the atmospheric variable?

The last, strictest standard is difficult to define and calculate, even in the case of ensemble hindcasts with no data assimilation, as described by Milroy et al.\textsuperscript{21}. We are not aware of any adaptations of those techniques to ensemble data assimilation.

Usage notes

Surface forcing files. CESM uses the coupler history (DATM surface forcing) files by reading their names and locations from “stream” files in the CASEROOT directory where the experiment is set up. Their names have the form “user_datm.streams.txt.prescribed_INST” where INST is an “instance number” (ensemble member, padded with 0s). In the context of a DART assimilation experiment, these stream files are created during the set up of the CASE from template files found in:

${DART}/models/{cice,clm,POP}/shell_scripts/streams.txt

In those directories there are also scripts with ‘setup’ in their names, which can be used to set up assimilation experiments, including the creation of the user_docn.streams.txt.prescribed_INST files. Before use, the coupler history files (e.g. f.e21.FHIST_BGC.f09_025.CAM6assim.011.cpl_0001.ha2x3h.2011.nc.gz) will need to be decompressed using ‘gunzip’.

Restart file sets. The restart file sets can be used to start a simple hindcast by decompressing one of them into an accessible “REFDIR” directory and setting CESM’s env_run.xml:

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure10.png}
\caption{Top; the posterior ensemble standard deviation (“spread”) of the meridional wind component (VS) on 2019-11-01-00000 at the model’s lowest level (8 hPa above the surface). The data range from $\sim 0.034$ to $\sim 10.6 \text{ ms}^{-1}$. Bottom; the same, but for the ensemble mean. The data range from $\sim -23.6$ to $\sim 23.8 \text{ ms}^{-1}$. The figure, including continental outlines, was drawn using ncview (version 2.1.7), which is open source software licensed under the Gnu General Public License version 3.}
\end{figure}
CONTINUE_RUN = FALSE
RUN_TYPE = hybrid
RUN_REFCASE = f.e21.FHIST_BGC.09_025.CAM6assim.011
RUN_REFPDIR = where the restart file set has been decompressed
RUN_REFDATE = the YYYY-MM-DD chosen as the date of the initial condition data. This can be a different year and day from the desired start date, but should be in the same month.
RUN_REFTOD = 00000

The restart file sets can be used to start an atmospheric assimilation by decompressing an ensemble of them into an accessible “REFDIR” directory and following the usual DART set up procedures, as outlined in the DART tutorials and scripts, such as $[DART]/models/cam-fv/shell_scripts/cems2_1/*setup*. This is not a trivial exercise, and will be done much more efficiently by becoming familiar with DART before attempting it.

Assimilation diagnostic files. If additional observation space diagnostics are needed, they can be derived from the f.e21.FHIST_BGC.09_025.CAM6assim.011.cam_obs_seq_final.YYYY-MM.tgz files using scripts and programs in DART, as outlined in Fig. 6. Some of those are described in “Observation sequence files”. In particular, program obs_diag can be rerun using different horizontal regions, time spans, vertical layers, etc. These are controlled by fortran namelist parameters in input.nml.obs_diag_nml.

DART has numerous Matlab© (.m) scripts to further process and display the contents of the NetCDF files produced by obs_diag.f90 and obs_seq_to_netcdf.f90. The latter creates files whose contents can be viewed as multiple linked frames with data selection capabilities. Several scripts display three-dimensional, rotatable renderings of the data. See DART’s Diagnostics page for illustrations and details.

Once the NetCDF files are created, software packages other than Matlab© could be used. In that case the Matlab© scripts can serve as helpful templates for dealing with the many issues which must be resolved to create useful pictures. Users have begun contributing Python code for the manipulation of DART diagnostic output. It is not as advanced as DART’s Matlab© environment, but we expect it to develop rapidly. Please contact us for the current status (dart@ucar.edu).

Land model time series. These NetCDF files can be evaluated and manipulated by the usual tools. The “h0” file variable time series are defined on the CAM lon-lat grid, so they can be easily displayed. The “h1” file variable time series have the CLM “pft” dimension (plant functional type), which is too large for display (≈ 800,000) without subsetting. There are many pfts in each grid box, distributed among the land surface types22.

Use cases. Several uses of this dataset have been described in previous sections:

▷ Use of the Surface Forcing Files in CESM (see Fig. 1 for an illustration).
▷ Restart File Sets describes initial conditions for hindcasts.
▷ assimilation innovations can be calculated from the data described in “Atmosphere model ensembles” and “Ensemble mean and spread files”
▷ Assimilation Files describes how to see and generate statistics describing the assimilation.
▷ Land Model Time Series describes the plant growth variables in the CLM5 history files (Table 9)
▷ Comparison of these reanalyses with others, but see comments in “Technical Validation”, or combination with them, as in the Multi-Reanalysis Ensemble v2.

This large dataset has a unique combination of an 80 member ensemble, 1° global resolution, 6-hourly frequency, and 9 year time span, which provides opportunities for robust statistical analysis and use as a machine learning training and verification dataset. The data differs from model generated training sets in that it is constrained to represent the atmosphere (and plant growth characteristics), rather than the model formulation.

The observation space diagnostics can be used to help identify biases in observation platforms. The dataset already contains biases of the reanalysis relative to a variety of observation types, as a function of season, time of day, height, and broad latitude regions. Further refinement of the influences on the biases can be generated, as needed.

Code availability. DART software is managed in github.com/NCAR/DART, where users can access the tag which was used to generate this reanalysis; “DS345.0”. The general web site for the version of CESM used here is http://www.cesm.ucar.edu/models/cesm2. The specific version can be found in github.com/kdraeader/cesm; the cesm2_1_forcing_rean branch. That branch includes a SourceMods tar file, which needs to be unpacked before building CAM6. There are minor changes to the CESM scripting to make it run more efficiently in ensemble mode. These are available in github.com/kdraeader/cime; in the cime_reanalysis_2019 branch. This cime needs to be imported into the CESM source code directory during the package build process, as described in the CESM documentation. Some of the csh scripts use NCO NetCDF operators, which are freely available. DART’s Matlab scripts are compatible with version R2018b, Update 5 (9.5.0.1178774), 64-bit (maci64), license number 473564.

Received: 26 February 2021; Accepted: 15 June 2021
Published online: 12 August 2021

References
1. Kalnay, E. Atmospheric Modeling, Data Assimilation, and Predictability (Cambridge University Press, 2003).
2. Izervinski, A. H. Stochastic Processes and Filtering Theory (Academic Press, 1970).
3. Daley, R. Atmospheric Data Analysis Vol. 2 (Cambridge University Press, 1993).
4. Anderson, J. L. et al. The data assimilation research testbed: A community facility. Bull. Am. Meteorol. Soc. 90, 1283–1296. https://doi.org/10.1175/2009BAMS2618.1 (2009).
5. DART-website. The data assimilation research testbed. http://www.image.ucar.edu/DAReS/DART/, https://doi.org/10.5065/D6WQ032J (Accessed on 03 Nov 2018) (2020).
6. Evensen, G. The ensemble Kalman filter: Theoretical formulation and practical implementation. Ocean Dyn. 53, 343–367. https://doi.org/10.1007/s10236-003-0026-9 (2003).
7. Fox, A. M. et al. Evaluation of a data assimilation system for land surface models using clm4.5. J. Adv. Model. Earth Syst. 10, 247–249. https://doi.org/10.1002/2018MS001362 (2018).
8. Zhang, Y.-F. et al. Assimilation of modis snow cover through the data assimilation research testbed and the community land model version 4. J. Geophys. Res. Atmos. 142, 1489–1508. https://doi.org/10.1002/2013JD021329 (2014).
9. Karspeck, A. R. et al. An ensemble adjustment Kalman filter for the cssm4 ocean component. J. Clim. 26, 7392–7413. https://doi.org/10.1175/JCLI-D-12-00402.1 (2013).
10. Schwartz, C. S., Romine, G. S., Sobash, R. A., Fossell, K. R. & Weisman, M. L. N' cars real-time convection-allowing ensemble assimilations, contributed to all of the above, and wrote the paper. J.L.A. and M.G. reviewed the manuscript.

Author contributions
J.L.A. motivated and supervised the project. T.J.H. wrote DART’s Matlab® scripts, helped choose appropriate CESM input files, evaluated monthly results, managed the git and github version control of DART and the reanalysis, and tested forcing files by applying them to CLM assimilations. M.G. evaluated monthly results, developed software to migrate them to a web site, and developed the inflation algorithm. B.K.J. analysed of the influence of the high resolution SST forcing on the assimilations, and tested forcing files by applying to POP assimilations. N.C. managed and reviewed DART software engineering. J.S. contributed significant efficiency improvement to CESM scripting. M.C. made system and resource modifications to ensure completion of the project. K.R. ran the assimilations, contributed to all of the above, and wrote the paper. J.L.A. and M.G. reviewed the manuscript.

Competing interests
The authors declare no competing interests.

Additional information
Correspondence and requests for materials should be addressed to K.R.

Publisher’s note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.
