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# gdess: A framework for evaluating simulated atmospheric $CO_2$ in Earth System Models

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## Summary

Atmospheric carbon dioxide ($CO_2$) plays a key role in the global carbon cycle and global warming. Climate-carbon feedbacks are often studied and estimated using Earth System Models (ESMs), which couple together multiple model components—including the atmosphere, ocean, terrestrial biosphere, and cryosphere—to jointly simulate mass and energy exchanges within and between these components. Despite tremendous advances, model intercomparisons and benchmarking are aspects of ESMs that warrant further improvement (Fer et al., 2021; Smith et al., 2014). Such benchmarking is critical because comparing the value of state variables in these simulations against observed values provides evidence for appropriately refining model components; moreover, researchers can learn much about Earth system dynamics in the process (Randall et al., 2019).

We introduce gdess (a.k.a., Greenhouse gas Diagnostics for Earth System Simulations), which parses observational datasets and ESM simulation output, combines them to be in a consistent structure, computes statistical metrics, and generates diagnostic visualizations. In its current incarnation, gdess facilitates evaluating a model's ability to reproduce observed temporal and spatial variations of atmospheric $CO_2$. The diagnostics implemented modularly in gdess support more rapid assessment and improvement of model-simulated global $CO_2$ sources and sinks associated with land and ocean ecosystem processes. We intend for this set of automated diagnostics to form an extensible, open source framework for future comparisons of simulated and observed concentrations of various greenhouse gases across Earth system models.

## Statement of need

Thorough evaluation of simulated atmospheric $CO_2$ concentrations—by comparing against observations—requires multiple diagnostics, metrics, and visualizations. During the past decade, such evaluations have utilized certain common methods, such as aggregating in situ measurements into latitude bands and detrending of multidecadal time series to investigate seasonal cycles (Chevallier et al., 2019; Jing et al., 2018; Keppel-Aleks et al., 2013; Liptak et al., 2017; Ott et al., 2015; Weir et al., 2021). However, the construction of diagnostics used in these evaluations has not been automated in an open-source tool available to the broader atmospheric modeling community. Thus, each modeling or analysis team has had to decide on and code their own preferred set of diagnostics, resulting in redundancies and potential inconsistencies among efforts.

Several software packages have been developed to streamline the application of diagnostics for ESM benchmarking. These tools share related functionality with gdess, and some have directly inspired the gdess design and our development approach. For example, the ESM Evaluation Tool (ESMValTool; Eyring, Righi, et al. (2016); Eyring et al. (2020)) has been used to generate specific figures from the literature, and we adopted the term *recipe* from its use by ESMValTool. Although ESMValTool includes a comparison of column-averaged $CO_2$ values as performed by Gier et al. (2020), gdess was created to provide specific $CO_2$ diagnostic methods and graphs that are not already provided as recipes in ESMValTool. gdess uses Observation Package (Obspack; Schuldt et al. (2020); Masarie et al. (2014)) data, which include atmospheric greenhouse gas observations from a variety of sampling platforms and data providers following the World Data Centre for Greenhouse Gases (WDCGG) protocol, so are widely used for stimulating and supporting carbon cycle modeling studies. These data have not been set up for use within ESMValTool, and as such would require additional development/configuration to work with ESMValTool. The International Land Model Benchmarking (ILAMB) System (Collier et al., 2018) excels at intercomparisons between multiple land models and has been used to benchmark inferred $CO_2$ concentrations against surface station measurements (Wu et al., 2020). In contrast to gdess, ILAMB provides the means to evaluate emulated results but not prognostic simulations for $CO_2$ (Keppel-Aleks, 2021).

## Design and data sources

gdess is written in Python ["version 3"; Python Core Team (2015); Van Rossum & Drake (2009)]. A comprehensive readme file and docstrings throughout the open source codebase (https://github.com/E3SM-Project/gdess) provide documentation and guidance, and Continuous Integration tests facilitate further code development and maintenance. Data variables are represented and handled in memory using xarray, an open-source Python package for working with labeled multi-dimensional arrays (Hoyer & Hamman, 2017).

As shown in Figure 1, gdess is organized into modular components. A *Collection* class encapsulates source-specific attributes and methods for each data source (described below) and each Collection inherits common attributes from a parent *Multiset* class. Each diagnostic recipe, defined in a separate module file (e.g., `surface_trends.py`), instantiates and uses Collection objects to handle the loading and pre-processing of data. Additionally, visualization functions (e.g., time-series, annual cycles) are accessible from any instance of a Collection or Multiset so that data sources can be inspected individually—i.e., without the need to run one of the comparative diagnostic recipes.

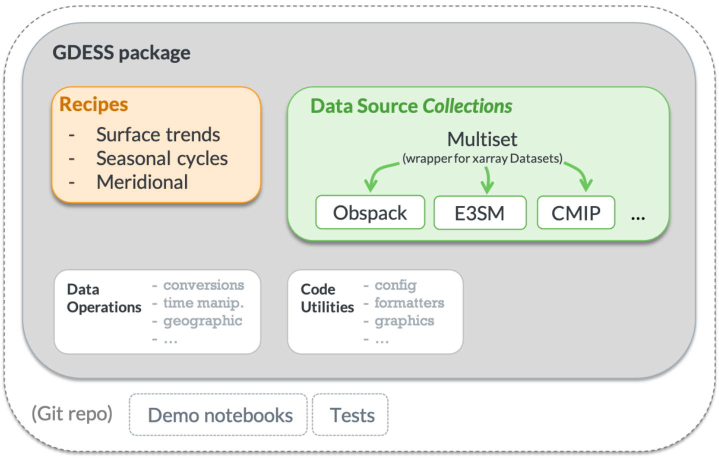


**Figure 1:** Schematic of the gdess code structure.

gdess can process data from three sources: Globalview+, CMIP, and E3SM. Data from surface observing stations must be retrieved from the NOAA Global Monitoring Laboratory (GML)

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Globalview+ version 6.0 Observation package (Obspack; Schuldt et al. (2020); Masarie et al. (2014)). In situ and flask measurements can be used from approximately 200 stations whose data in Obspack spans at least a 12 month period (Figure 2).

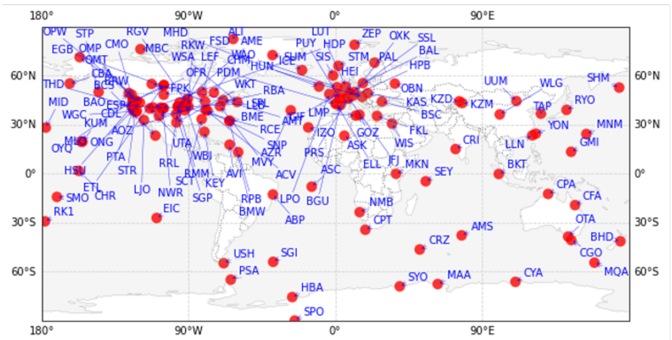


**Figure 2:** Global map showing surface observing station locations (red circles) and their three-letter site codes, as recorded in Obspack and used in gdess.

We distinguish between the model results from two different sources: (i) simulations by the Energy Exascale Earth System Model (E3SM), and (ii) other Earth system models participating in the latest, Version 6, Coupled Model Intercomparison Project (CMIP6). E3SM is a global modeling system composed of multiple coupled subcomponent models: atmosphere, ocean, land, ice (Burrows et al., 2020; Golaz et al., 2019). In this study, our focus is on evaluating $CO_2$ mole fractions in the atmospheric component, which is called the E3SM atmosphere model (EAM) and which has been described in detail by Rasch et al. (2019).

CMIP6 organizes the setup, experimental design, and intercomparisons of simulations performed using numerous global climate models. Data from CMIP6 are accessed either via locally stored files—downloaded directly from Earth System Grid Federation (ESGF) data nodes—or programmatically via the *intake-esm* package, which is a gdess dependency maintained as part of the *Pangeo* project. By default, comparisons in gdess use data from the 'esm-hist' experiment, which contains $CO_2$ emission-driven simulations that span the period of 1850 to 2014—i.e., an "all-forcing simulation of the recent past with atmospheric $CO_2$ concentration calculated" (Eyring, Bony, et al., 2016). We expect model output from any CMIP6 experiment could be used by specifying the appropriate data identifier or file location, although additional testing would be needed to confirm expected behavior.

# Functionality

This section describes and provides example output from the three diagnostic recipes implemented in gdess. These recipes can be initiated either from a terminal or from within a running Python kernel. The command-line interface consists of the gdess command, followed by the type of recipe, and then options for each recipe—e.g., which observing station(s) to use for comparison. Within a Python kernel, options are specified via a dictionary object.

### Multidecadal trend

Skillful simulation of the historical multidecadal trend in atmospheric $CO_2$ is a necessary condition for an ESM to be an effective tool for conducting climatological projections and analyses. The research questions one might address with this diagnostic recipe (see example output in Figure 3) include: What are the long-term biases in the model simulation? How does the simulated increase in $CO_2$ mixing ratios compare to surface measurements?

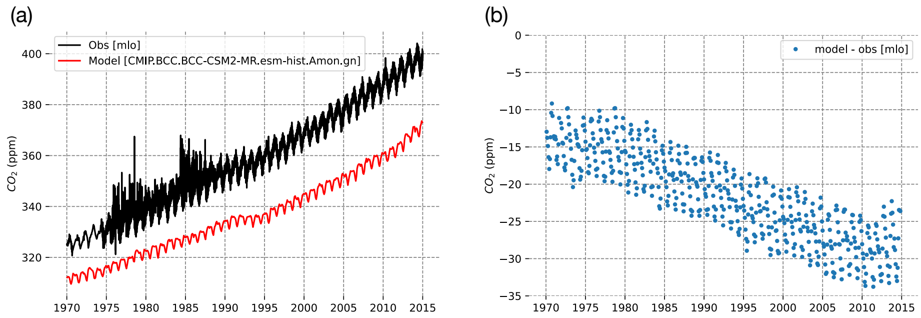


**Figure 3:** Example output of the `surface_trends` recipe, showing (a) individual time series and (b) differences between simulated and observed concentrations of surface-level atmospheric $CO_2$ at the Mauna Loa Observatory, Hawaii (MLO).

### Seasonal cycle

Because of the substantial impact primary production and respiration have on $CO_2$ concentrations, evaluating the seasonal cycle at a given location can help disentangle the effects of biological from physical processes. The seasonal cycle can be quantified by "the projection of an atmospheric time series onto a suitably defined subset of orthogonal basis functions, the choice of which depends on the length of the series involved" (Straus, 1983). For computing the seasonal cycle, we detrend the time series by fitting a function composed of both polynomial and harmonic terms, following the procedure of Sweeney et al. (2015) and originally proposed by Thoning & Tans (1989). Example output of the `seasonal cycle` recipe is shown in Figure 4.

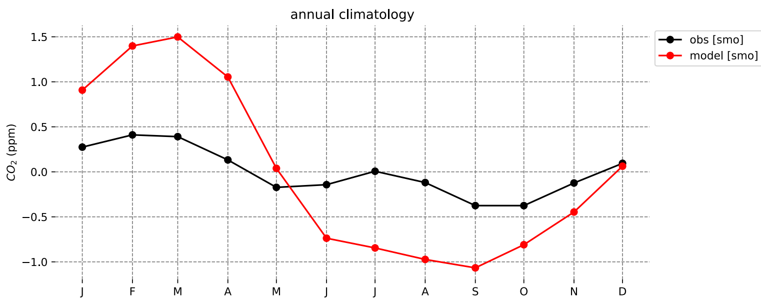


**Figure 4:** Example output of the `seasonal_cycle` recipe, comparing annual climatologies of surface atmospheric $CO_2$ concentrations at the American Samoa Observatory, Tutuila Island (SMO).

### Meridional gradient

By comparing $CO_2$ concentrations across observing sites distributed globally, we can assess whether simulated transport and mixing is skillfully reproducing spatial gradients. For instance, the surface $CO_2$ flux signals at lower latitudes (30-45N) are moved to northern boreal latitudes and also to the south by large scale circulation. Spatial analysis can reveal evidence of southward movement toward (sub)tropical convection that becomes mixed with Hadley circulation or northward movement toward midlatitude synoptic weather patterns and the Ferrell circulation (Denning et al., 1999; Schuh et al., 2019; Stephens et al., 2007). Figure 5 shows example output of the `meridional` recipe.

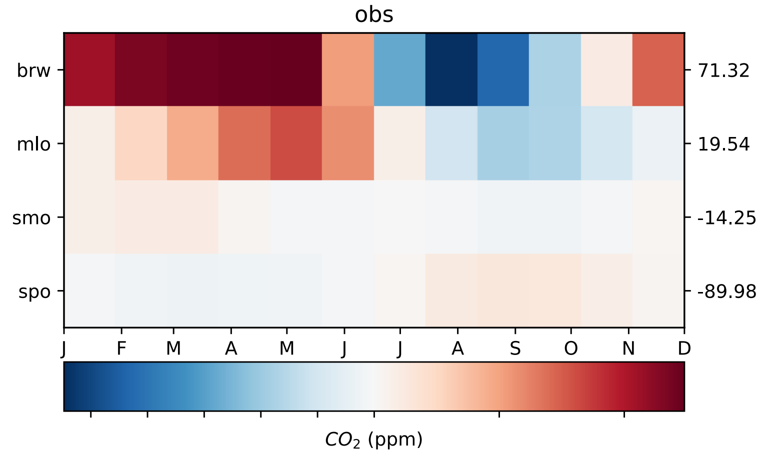


**Figure 5:** Example output of the `meridional` recipe, comparing the seasonal cycle across latitudes, at locations of user-specified surface stations.

## Outlook

Currently, `gdess` is helping to assess simulations using the biogeochemistry configuration of E3SM, with the aim of exploring carbon-climate interactions. In addition to the three implemented recipes (multidecadal trends, seasonal cycles, and meridional gradients), current development includes two other methods—by which $CO_2$ was also evaluated by Keppel-Aleks et al. (2013)—vertical gradients and interannual variability. Future releases may evaluate vertical gradients using aircraft data from Globalview+ Obspack, include satellite data, and extend to data for other greenhouse gases, such as methane.

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## Author contributions

D.K., K.C., B.H., and S.B. initially conceived the study. D.K. was the main code contributor of the gdess software and wrote the initial version of the paper. S.F. contributed to code testing. S.F., B.H., and S.B. ideated the experiment examples and priorities. All authors discussed the results, commented, and contributed to writing of the final version of the paper. K.C. supervised the study.

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