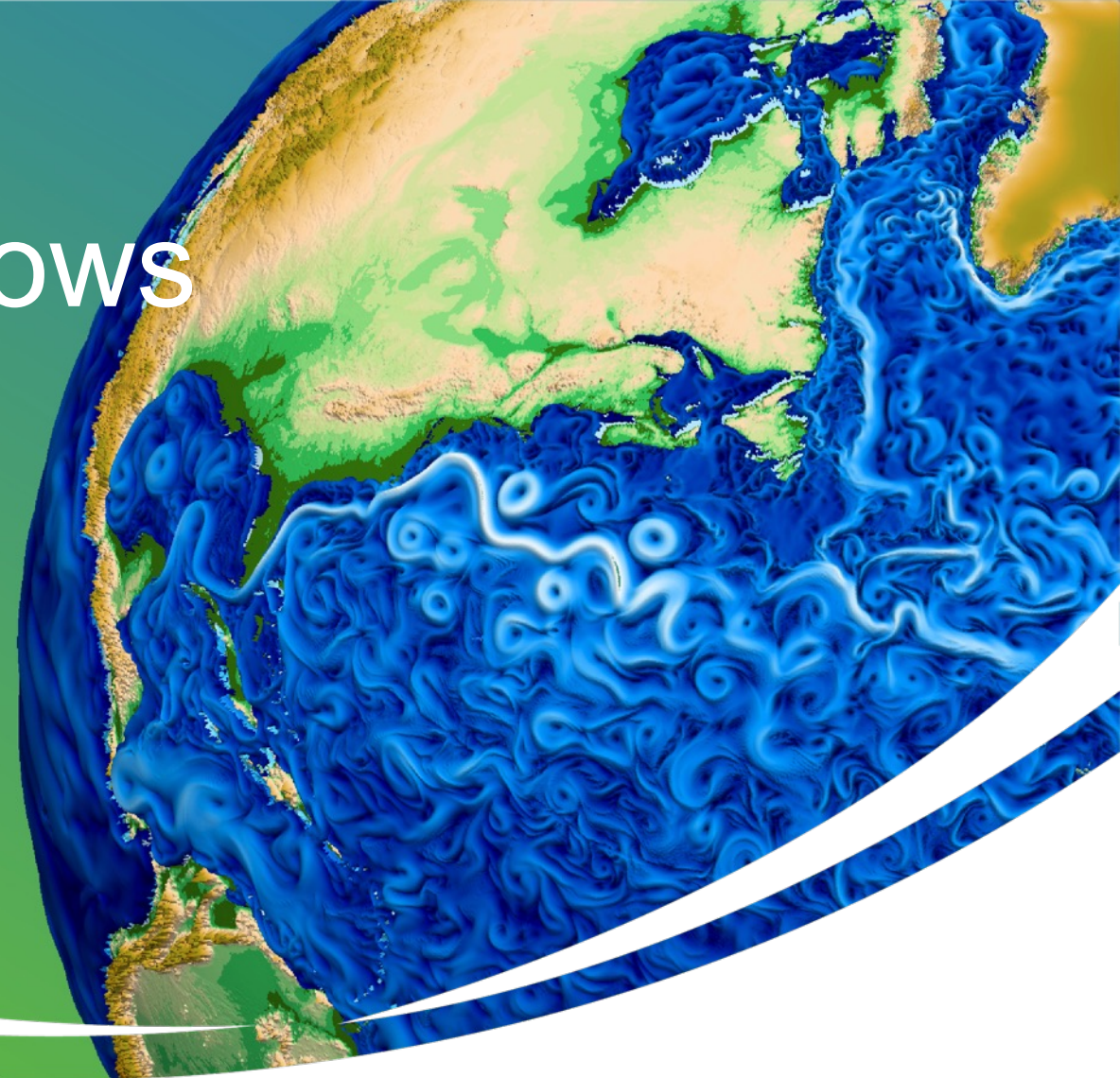


Post-processing Workflows and Tools for E3SM

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Jim Fourcar, Jason Boutte, Rob Jacob

CESM Workshop
Software Engineering Working Group session
June 14th, 2023



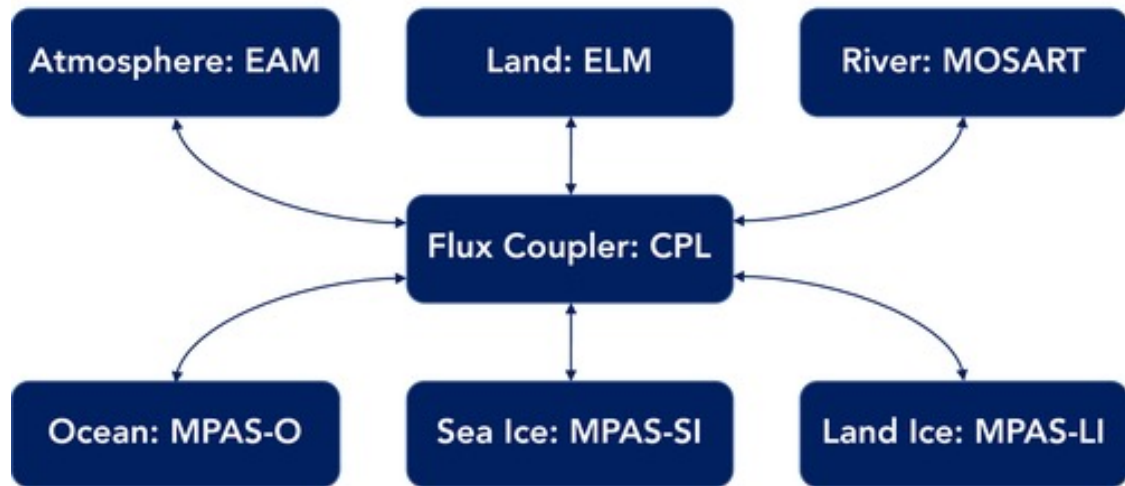
This work is performed under the auspices of the US DOE by the Lawrence Livermore National Laboratory under contract no. DE-AC52-07NA27344. LLNL-PRES-850133



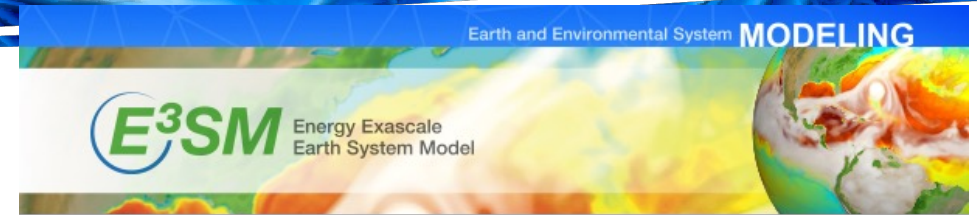
Brief Introduction: E3SM

- Focused on Department of Energy (DOE) missions and DOE leadership computing facilities.
- E3SM v1 was branched off CESM1.0.

Energy Exascale Earth System Model

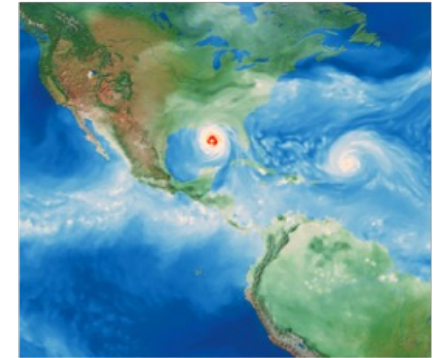


- The Infrastructure Group supports tools to run E3SM and to post-process and analyze the data.



E3SM: The Energy Exascale Earth System Model

Scientists are addressing major research areas in earth system science by developing and applying high-fidelity models that represent earth system changes to improve understanding of the significant drivers, feedbacks, and uncertainties within the integrated earth system. This research provides information needed for effective energy and connected infrastructure planning.



The Energy Exascale Earth System Model (E3SM) project is a state-of-the-science earth system modeling, simulation, and prediction project that optimizes the use of U.S. Department of Energy (DOE) laboratory resources to meet the science needs of the nation and the mission needs of DOE.

KEEP UP TO DATE ON E3SM

E3SM publishes news, feature stories and technical information on its website. The E3SM project also publishes *Floating Points*, a quarterly email newsletter. Follow the links below to get to know more about E3SM and to subscribe to E3SM's newsletter.

- Subscribe to our newsletter by emailing your contact information to listserv@listserv.llnl.gov with "subscribe e3sm-news" in the body of the email
- Visit our website: www.e3sm.org
- Read our project news: <https://e3sm.org/about/news>
- Check out our most recent publications: <http://bit.ly/E3SMPublications>
- Review our research highlights: <http://bit.ly/E3SMHighlights>

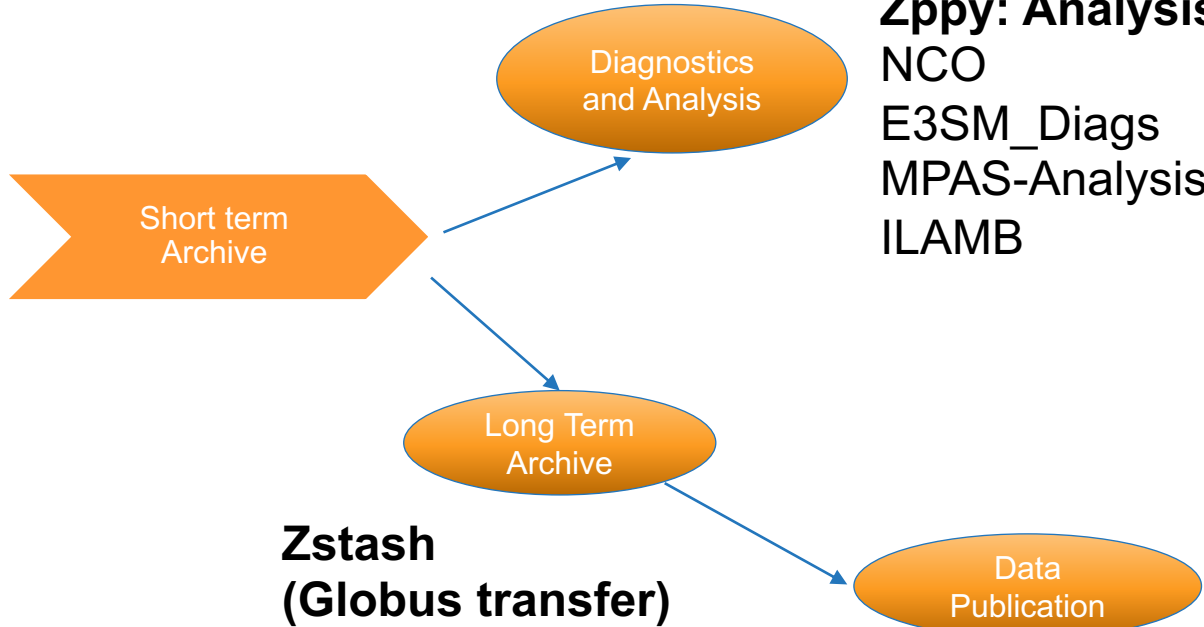


Post-processing for Earth System Models

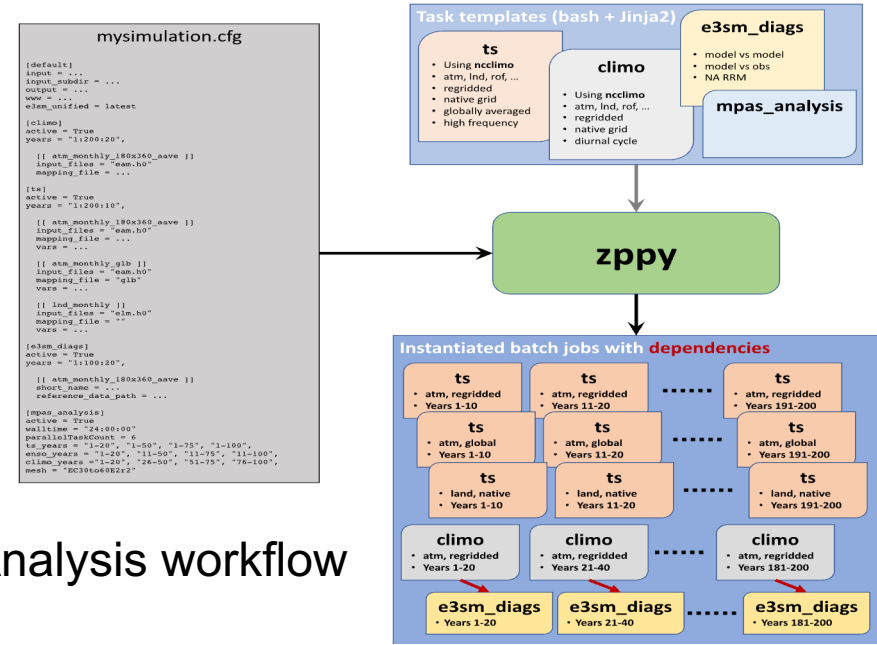
- Goal: facilitate model data reformation and distribution for scientific discovery
- End products:
 - From **core post-processing**:
 - Time series NetCDF files (e.g. CMIP format)
 - Climatology NetCDF files
 - Standard **diagnostics** results

Data are archived on tape/disk storage or distributed through web servers (i.e. ESGF)

E3SM post-processing workflows

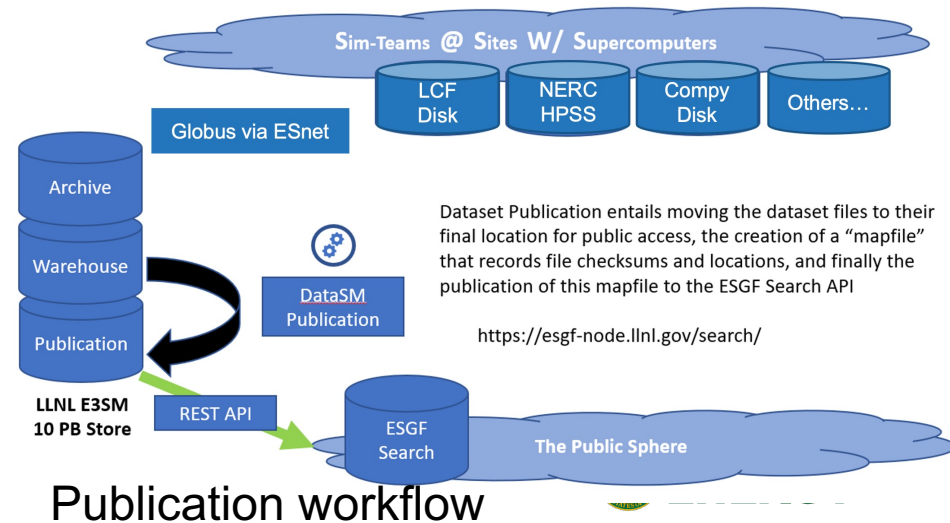


Zppy: Analysis workflow
NCO
E3SM_Diags
MPAS-Analysis
ILAMB



Analysis workflow

Data state machine: Publication workflow
File extraction from zstash archive (not automated)
Post processing (NCO, e3sm_to_cmip6)
Data publication to ESGF
Data quality checks and status logging

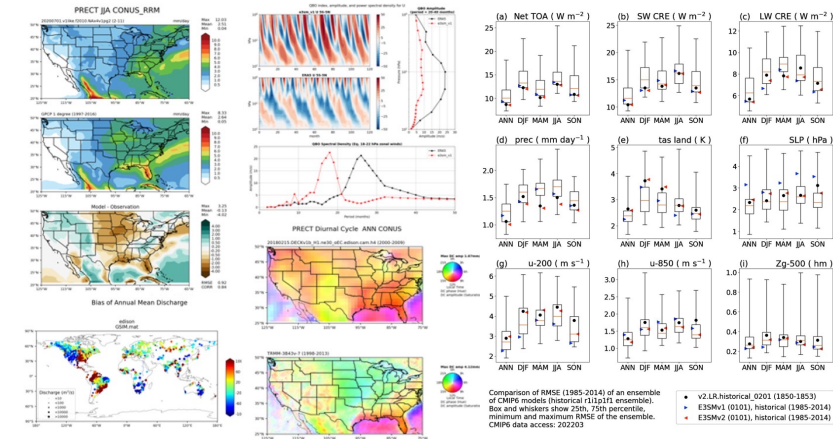


Publication workflow

E3SM Analysis tools

Major Tools included in standard analysis workflow:

- **NCO:** Regidding, Climatology Generation and Timeseries Extraction, support **all E3SM components**
- **E3SM-Diags:** Diagnostics package for **Atmosphere**, extending the support to **Land and River**
- **MPAS-Analysis:** Diagnostics package for **Ocean and Sea-ice**
- **E3SM-Unified:** Conda package for distributing all the above
- **Zppy:** Post-processing tool chain to automate most commonly analysis



E3SM Diags (C. Zhang et. al 2023)

More tools used in E3SM evaluation /connected to E3SM:



MDTF diagnostics

MPAS-Analysis Diagnostics: Ocean

MPAS
Model for Prediction Across Scales

Run: 3DGM

Quick Links

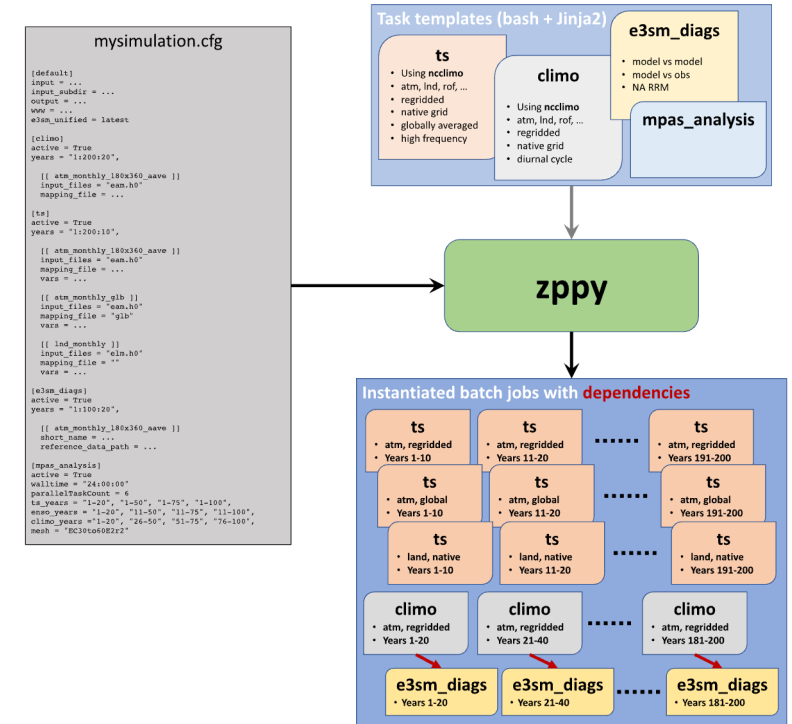
Global Mixed-Layer Depth	Global Sea Surface Temperature	Global Sea Surface Salinity	Global Sea Surface Height	Global OHC Anomaly

Antarctic Potential Temperature	Antarctic Salinity	Antarctic Potential Density	Antarctic Mixed Layer Depth	Antarctic Zonal Velocity

Zppy enables orchestration of post processing tasks

Goal: Speed up the post-processing by automating **commonly performed analysis tasks**.

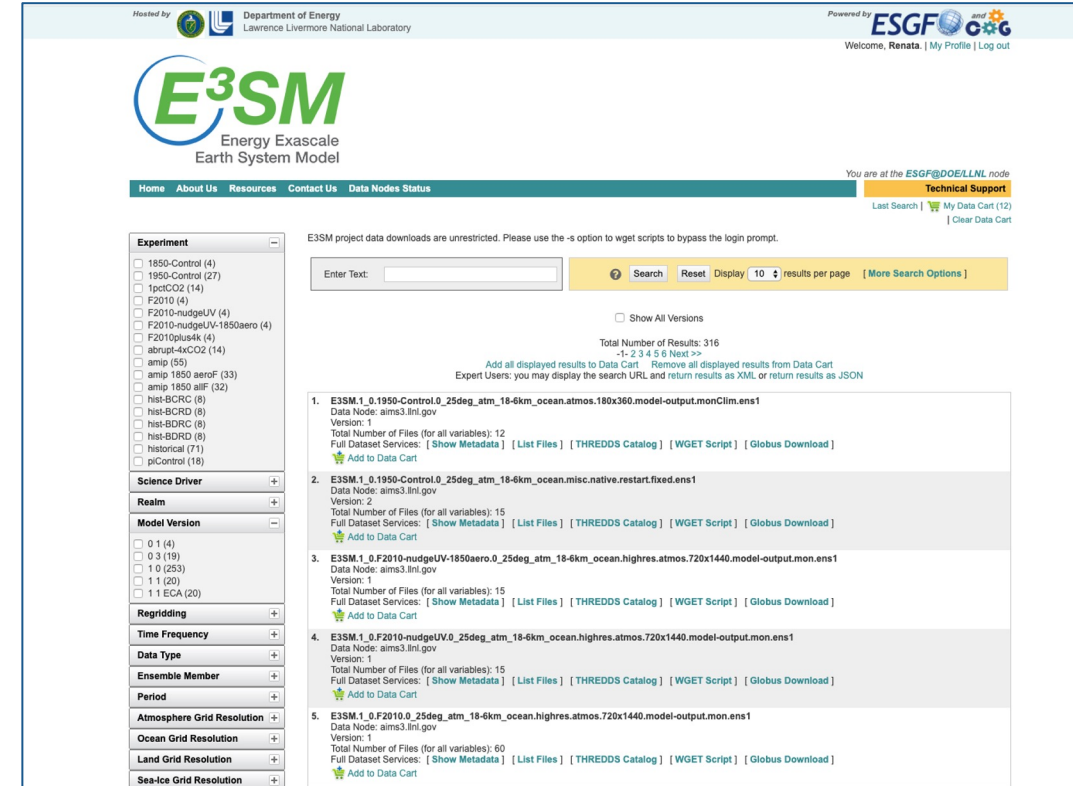
- Built around tasks:
 - time series/climatology with NCO,
 - E3SM Diags or MPAS-Analysis or ILAMB.
 - Generating global mean time series and plot.
- A framework to simplify tools use, esp. for long simulations.
- A single configurable file
- Zppy parses the configuration file, handles dependencies and generates/submit batch jobs for execution by SLURM.



<https://e3sm-project.github.io/zppy>

E3SM Data Publication Tools

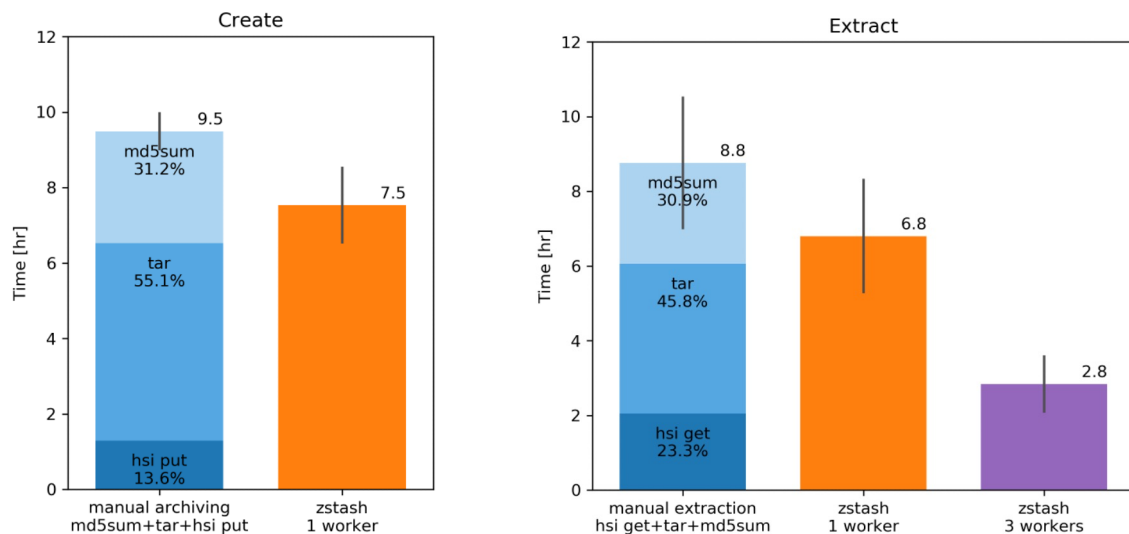
- For all production simulations:
 - A copy of uniformly archived (zstashed) data on **NERSC HPSS**
 - **Native files publication + CMIP-formatted subset to ESGF**
- Tools for data publication :
 - **Zstash**: long term archiving solution for E3SM
 - **E3sm_to_cmip**: Reformat native E3SM output to adhere to strict CMIP6 data protocols and format
 - **Data state machine**:
 - Automated post-processing
 - Automated status reports, data version control and data quality checks
 - Make data available through ESGF



The screenshot shows the E3SM Data Portal interface. At the top, it is hosted by the Department of Energy, Lawrence Livermore National Laboratory, and powered by ESGF. The main header includes the E3SM logo and navigation links: Home, About Us, Resources, Contact Us, and Data Nodes Status. A search bar is present with a search button and options for results per page (10) and more search options. Below the search bar, there are several filter sections: Experiment (with checkboxes for various simulation types like 1850-Control, F2010, etc.), Science Driver, Realm, Model Version, Regridding, Time Frequency, Data Type, Ensemble Member, Period, Atmosphere Grid Resolution, Ocean Grid Resolution, Land Grid Resolution, and Sea-Ice Grid Resolution. The main content area displays a list of data products, each with details such as Data Node, Version, Total Number of Files, and links for metadata, files, and download options.

zstash: HPSS long-term archiving tool

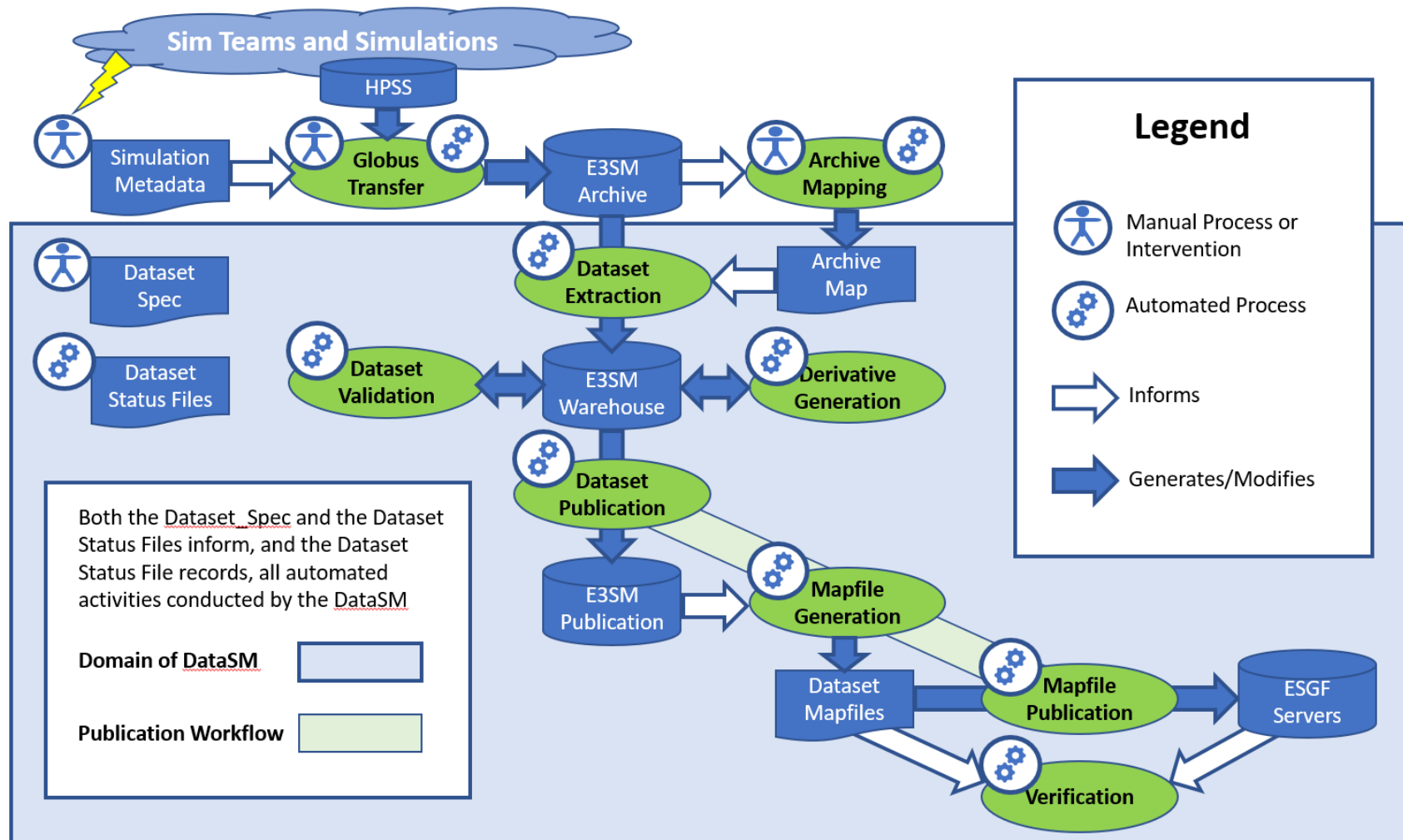
- A Python tool for long-term HPSS archiving of E3SM simulations with features:
 - **Standard tar files** generated locally before transfer to HPSS
 - **Checksums (md5)** are computed *on-the-fly* during archiving and **verified** on extraction
 - Metadata stored in a sqlite3 index **database**, enabling **faster retrieval** for target files
 - **Parallel extraction and verification** for increased performance
 - Enables **automated Globus transfer** to move archived files to another system



Performance comparison for zstash 'Create' and 'Extract'.
Blue: manual operations with separate md5sum, tar and hsi steps.
Orange: comparable combined operations with zstash with 1 worker.
Purple: zstash with 3 workers (parallel operation)

Performance data for a 4 TB archive consisting of more than 13,000 files.
 Mean and range of three realizations on NERSC's Data Transfer Nodes.

E3SM Data Publication Workflow



Handling Large Size Data

Dataset Validation ensures “Clean native data”:

1. Uncover missing files (in time to re-request the data if possible)
2. Uncover (and often correct) overlapping files and mismatched time-indices

Published data size on ESGF

- 1551 TB total to E3SM Project Space
- 42 TB total to CMIP6

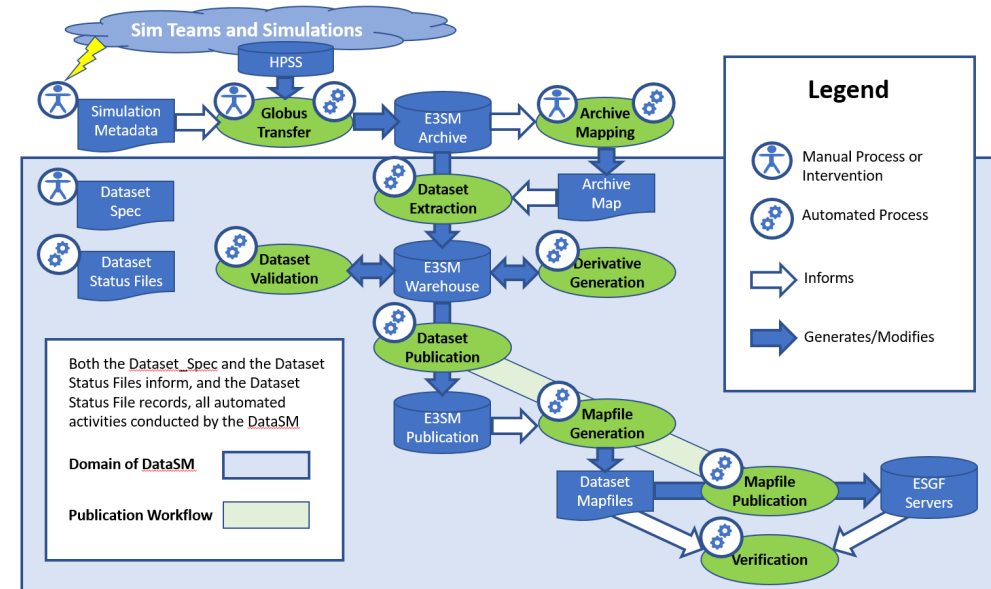
A temporary warehouse/staging area with unified tree breakout structure

1. Various-formatted datasets are re-grouped (short-archive, h tape #)
2. Host repaired datasets when needed
3. Temp holding of (native+derived) data until publication is authorized.

Dataset Status Files tracks status of dataflow per-dataset

Example:

<timestamp>:GlobusTransfer:Engaged
<timestamp>:ArchiveMapping:Pending
<timestamp>:ArchiveExtraction:Pending



Future work

- Workflows are not end-to-end:
 - The data publication and analysis workflows can be consolidated
 - Auto generation of simulation documentation page is desired
- Larger size dataset challenge:
 - Reduce variables from production runs
 - Explore using data compression, (~100 TB of output per simulated year for 3km SCREAM)
 - Performance enhancement for tools.

Post-Processing tools

- Goal: Support infrastructure for E3SM and external projects to post-process and analyze the data.
- Immediately after the run:
 - Restart, short-term archive with **CCS** (jointly developed with NCAR)
 - Post process with **zppy**
 - Archive to disk with **zstash**
- Platform support tools:
 - E3SM analysis environment: **e3sm_unified**
 - Provide supported Machine information: **Mache**
- Diagnostics and Analysis
 - Regridding and generate time series/climatology: **NCO**
 - Atmosphere, land, river diagnostics: **E3SM Diags.**
 - Ocean and sea-ice diagnostics: **MPAS-Analysis**
 - New python library for climate data analysis: **xCDAT** (jointly developed with RGMA funded SEATS project)
- Data Publication
 - Reformat E3SM data to CMIP: **e3sm_to_cmip**
 - Workflow tool for ESGF publication: **Data state machine**

***Most are Python Tools;
Open development on GitHub;
Inquiries and collaboration are welcome!!***



**Questions?
(and thank you!)**