CESM CMIP6 Data Workflow

Sheri Mickelson
CISL/TDD/ASAP
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CESM Workflow Refactoring Team

- Ben Andre
- Alice Bertini *
- John Dennis
- Jim Edwards
- Mary Haley
- Jean-Francois Lamarque
- Michael Levy
- Sheri Mickelson *
- Kevin Paul *
- Sean Santos
- Jay Shollenberger *
- Gary Strand
- Mariana Vertenstein

(* Developer)
CMIP5 Workflow

Model Run

CESM Model Run

Post-Processing

Time Series Conversion (NCO)

Diagnostics (NCO/NCL)

CMOR

Publication

Push to ESGF
Lessons We Learned From CMIP5

• CESM was the first model to complete their simulations, but the last to complete publication. Why?
  – All post-processing was serial
  – Workflow was error prone and took time to debug
  – Too much human intervention was needed between post-processing steps
Plans for CMIP6 (Preliminary)

- Participate in 26 MIPS
- **Low Resolution: 1° atm, 1° ocn**
  - Throughput: 14.5 simulated years per wall clock day
  - Cost: ~2,000 core hours per simulated year
  - Total estimated cost: 150 million core hours
- **High Resolution: 25km atm, 1° ocn**
  - Throughput: 1.84 simulated years per wall clock day
  - Cost: ~215,000 core hours per simulated year
  - Total estimated cost: 350 million core hours
- **Data sizes:**
  - Raw size: ~12 PB
  - Published: ~6 PB = we will have to process 5TB a day for 3 years
To quote Jim Kinter, how are we going to post-process the flood of data from CMIP6?

Our current boat won’t be able to process the flood of data
New CESM/CMIP6 Workflow

- We have been examining the individual pieces of the workflow and improving it where necessary
  - Increasing performance: Adding parallelization into the workflow
  - Reducing Human Intervention: Adding in automation
  - Project Management: more formal approach
New CESM/CMIP6 Workflow

Model Run

Post-Processing
- Time Series Conversion (PyReshaper)
- New Data Compliance Tool
- Re-Designed Diagnostics (PyAverager)

Publication
- Push to ESGF (Improved process)

Automated Task Submission to Machine Queue

Experiments Update Their Status in Run Database
New CESM/CMIP6 Workflow

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Post-Processing

Publication

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The previous method worked in serial using NCO.

This was one of the most expensive CMIP5 post-processing steps.
PyReshaper Details

The PyReshaper is a light weight custom Python concatenation tool

• We chose Python for its flexibility and its fast development rate.

• For easier portability, we rely on only 3 packages
  – PyNIO (Python version of the NCL I/O utilities)
  – mpi4py (Package used for parallelization)
  – NumPy (Used for data storage)
PyReshaper Parallelization Scheme

Each rank is responsible for writing one (or more) time-series variables to a file.
### Time-Slice to Time-Series Conversion

#### Timing Statistics

<table>
<thead>
<tr>
<th>Existing Method (NCO)</th>
<th>Time (per MIP per Year)</th>
<th>Average Throughput (per run)</th>
<th>Throughput per Calendar Day</th>
</tr>
</thead>
<tbody>
<tr>
<td>1° atm, 1° ocn</td>
<td>225 minutes</td>
<td>1.85 MB/sec</td>
<td>0.15 TB</td>
</tr>
<tr>
<td>25km atm, 1° ocn</td>
<td>478 minutes</td>
<td>4.85 MB/sec</td>
<td>0.40 TB</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>New Method (PyReshaper)</th>
<th>Time (per MIP per Year)</th>
<th>Average Throughput (per run)</th>
<th>Throughput per Calendar Day</th>
</tr>
</thead>
<tbody>
<tr>
<td>1° atm, 1° ocn</td>
<td>4 minutes</td>
<td>104 MB/sec</td>
<td>8 TB</td>
</tr>
<tr>
<td>25km atm, 1° ocn</td>
<td>8 minutes</td>
<td>290 MB/sec</td>
<td>23 TB</td>
</tr>
</tbody>
</table>

- Conversions were ran on Yellowstone using 4 nodes/4 cores (16 cores total)
- The PyReshaper increases performance by 50-60x and achieves better machine utilization
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Experiments Update Their Status in Run Database
Original Diagnostic Packages

- **Work focusing on redesigning**
  - Our 4 main component Diagnostic Packages
  - ILAMB Package

- **The Original packages**
  - Contain top level control scripts
  - Create climatology files with NCO tools
  - Create hundreds of plots with NCL scripts
  - Create web pages that allow users to browse through plots
  - The ILAMB Package creates climos and plots with NCL

- **Problems:**
  - Contain no parallelization
  - They often break at high resolution
  - They do not work with time series files
Re-Design of Diagnostic Packages

• Add in Parallelization
  – Instead of NCO, use the PyAverager to create the climatology files in parallel
  – Run the NCL plotting scripts in parallel

• Allow the packages to work with either time slice or time series files
PyAverager Details

• A light weight custom Python averaging tool
  – Parallelizes over variables and averages
  – Depends on PyNIO, mpi4py, and NumPy

• Computes temporal averages
  – Seasonal, Yearly, Annual, Monthly (weighted optional)

• Can concatenate in parallel
PyAverager Parallelization Scheme

- **Time Averaged Climatology File**
- **Time Series Files**
- **Averages to Compute**
- **InterCommunicator 1**
- **InterCommunicator 2**
- **InterCommunicator 3**

Diagram shows the parallelization scheme with multiple ranks and communicators.
PyAverager Parallelization Scheme

Time Averaged Climatology File

Time-Series Files

Averages to Compute

Time Averages (Internal Memory)

Computational & Information Systems Laboratory

InterCommunicator 1

InterCommunicator 2

InterCommunicator 3
PyAverager Parallelization Scheme

Time-averaged climatology file

Time-series files

Averages to compute

InterCommunicator 1

InterCommunicator 2

InterCommunicator 3
PyAverager Parallelization Scheme

Averages to Compute

Time-Series Files

Time Averages (Internal Memory)

Time Averaged Climatology File

InterCommunicator 1

InterCommunicator 2

InterCommunicator 3
PyAverager Performance Using CESM Data

Time to compute climatology files for 10 years of CESM monthly time slice files. The PyAverager ran on 120 cores on yellowstone.

140x overall performance improvement

- ATM-SE: 14x
- ICE: 28x
- LND: 36x
- OCN: 240x
- Total: 140x

CESM Model Component

Time (minutes) log scale

0.1

1

10

100

1000
Diagnostic Performance

Performance Comparison Across Diagnostic Packages

All parallel diagnostics were ran on 16 Yellowstone cores.
Making Our Tools General Enough to Handle Other Modeling Data

- Both the PyReshaper and the PyAverager can operate on non-CESM data
- Because we chose PyNIO for our I/O library, we can read in any data type that NCL can handle
PyAverager Performance Using Data From Other Models

CMIP5/AMIP monthly data. 5 seasonal and 12 monthly averages were computed over 29 years for 5 variables. The PyAverager was ran on 36 cores on yellowstone. The combined operation option was used for CDO.
New CESM/CMIP6 Workflow

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CESM Model Run

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Push to ESGF (Improved process)

Experiments Update Their Status in Run Database

Automated Task Submission to Machine Queue
New Data Compliance Tool

• Main Goals
  – Provide a simple user interface
  – Add data transformation and calculator abilities
  – Add parallelization to increase performance (this was another bottleneck in CMIP5)

• We are using similar techniques that were used by the PyReshaper and PyAverager
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CESM Model Run

Experiments Update Their Status in Run Database

Updated Status in Run Database
ESGF Publication

- Move the data staging, directory structuring, and versioning responsibilities into the new compliance tool
- Streamline the submission process
- ESGF currently undergoing a major overhaul to address performance and reliability concerns
- New version of TDS (Unidata)
  - Better memory and resource management
- We will be setting up a test ESGF node to test new features and to access this portion of the workflow
New CESM/CMIP6 Workflow

Automated Task Submission to Machine Queue

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Requirements for an Automated Workflow Management System

• We need a light weight and portable option
  – Needs to run on everything from laptops to shared supers per CESM user community requirements

• We evaluated Cylc and Rocoto
  – Both are very impressive, but lacked the portability that CESM required

• Since we have already developed an experiment database that we can extend, we only lacked a task scheduler
Our New Workflow Management System

- The system evaluates user options and submits workflow to the machine’s queue as dependency jobs.
- The management system will automatically:
  - Run the PyReshaper after a select number of years has passed.
  - Detect if and when to run diagnostics based on user selected date ranges.
  - Run the data compliance tool after the PyReshaper successfully finishes.
New CESM/CMIP6 Workflow

Automated Task Submission to Machine Queue

Model Run

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Experiments Update Their Status in Run Database
**Current Run Database**

Basic Catalog of Experiment Information

- Users manually enter experiments into the DB
Current Run Database

Basic Catalog of Experiment Information

- Users manually enter experiments into the DB
- Contains basic search utilities and search filters

![Search Filter Options](chart.png)

Displaying experiments [1 - 25] out of 1767

<table>
<thead>
<tr>
<th>ID</th>
<th>Case Name</th>
<th>Diags</th>
<th>Pubs</th>
<th>Type</th>
<th>Comset</th>
<th>Resolution</th>
<th>Machine</th>
<th>Request Date</th>
<th>Status</th>
<th>Assigned</th>
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</thead>
<tbody>
<tr>
<td>1684</td>
<td>b.e11.B1850C5CN.ne30_g16.control.003</td>
<td>Diags</td>
<td>Pubs</td>
<td>EXP</td>
<td>TBD</td>
<td>TBD</td>
<td>TBD</td>
<td>2013-06-27</td>
<td>Running</td>
<td>TBD</td>
</tr>
<tr>
<td>1667</td>
<td>b.e12.B1850C5CN.ne30_g16.control.002</td>
<td>Diags</td>
<td>Pubs</td>
<td>EXP</td>
<td>B_1850-2000_CAM5_CN</td>
<td>ne30mp4_gx1v6</td>
<td>yellowstone</td>
<td>2013-05-09</td>
<td>Running</td>
<td>TBD</td>
</tr>
</tbody>
</table>
Current Run Database

Basic Catalog of Experiment Information

- Users manually enter experiments into the DB
- Contains basic search utilities and search filters
- Lists available experiments

![CIESM Experiment Database Image]
Enhancements to the Run Database

- Automating the process of adding an experiment to the database
- Adding a separate section for CMIP6 experiments
- All experiments will update their run status to the database (simulation progress/color coded run status)
- CMIP6 timeline views
- Resource tracking (i.e. available disk space)
- Optional link to diagnostic web pages
Project Timeline
January 2014 – June 2016

- PyReshaper *
- PyAverager *
- Automated Job Control *
- Diagnostic Packages
- Experiment Database
- Data Compliance Tool
- Incrementally Testing the Workflow
- Evaluate ESGF

* Completed

- September 2015
- June 2016 Release of CESM2.0
Conclusions

• CMIP5 stressed our workflow and showed us where we needed improvements

• We are introducing incremental changes and adding them into our current workflow and testing them before CMIP6 starts

• Our new tools provide significant performance improvements
  – PyReshaper: 50-60x speedup
  – PyAverager: 14-240x speedup
Conclusions Continued

• Our new Python tools are general across all models, do not have many dependencies, and can be easily integrated into a workflow

• We continue to building additional tools that will improve our workflow
Questions?

Python Tool Availability

Github
• https://github.com/NCAR-CISL-ASAP/PyReshaper
• https://github.com/NCAR-CISL-ASAP/pyAverager
• https://github.com/NCAR-CISL-ASAP/ASAPPyTools

PIP
• pip install PyReshaper
• pip install pyAverager
• pip install ASAPTools

Contact Information
mickelso.at.ucar.edu
https://www2.cisl.ucar.edu/tdd/asap/parallel-python-tools-post-processing-climate-data