Optimizing Workflow for CESM

Sheri Mickelson
ASAP/TDD/CISL
CSEG/CGD
Thanks to all of the CESM workflow refactor team for their work and guidance

• 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
Different people responsible for different tasks required time consuming communication

Lack of parallelization in post-processing causes the post-processing to take longer than the experiment to runs
Goals For New CESM/CMIP6 Workflow

• Improve orchestration of the workflow and add in automation
• Examine the individual pieces of the workflow and improve where necessary
• Add parallelization into the workflow
• Create more formal project management tools
New CESM/CMIP6 Workflow

Model Run

Post-Processing

- Time Series Conversion (PyReshaper)
- Re-Designed Diagnostics (PyAverager for climos)
- New Data Compliance Tool

Publication

- Push to ESGF (Improved process)

Automated Task Submission to Machine Queue

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

Model Run

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

Publication
- Push to ESGF (Improved process)

Automated Task Submission to Machine Queue

Experiments Update Their Status in Run Database
Simple diagram, but a lot going on behind the scenes ...

Orchestration and automating the submission of CESM and post-processing tasks

• Users are able to turn post-processing tasks on/off and select date ranges to process

• Based on selections, post-processing jobs will automatically be submitted to the queuing system
New CESM/CMIP6 Workflow

- Model Run
  - CESM Model Run

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

- Publication
  - Push to ESGF (Improved process)

Automated Task Submission to Machine Queue

Experiments Update Their Status in Run Database
Enhancements to the Run Database

• There will be a separate section for CMIP6 experiments
• All experiments will update 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
New CESM/CMIP6 Workflow

Model Run

Post-Processing
- Time Series Conversion (PyReshaper)
- Re-Designed Diagnostics (PyAverager for climos)
- New Data Compliance Tool
- Push to ESGF (Improved process)

Publication

Automated Task Submission to Machine Queue

Experiments Update Their Status in Run Database
Re-Design of Diagnostic Packages

• Can be automatically ran as part of a CESM run, but they still maintain the capability to ran standalone
  – Configured through XML Options
  – Sets up a Python Virtual Environment for users

• Instead of NCO, use the PyAverager to create the climatology files (from either time slice or time series files)

• Runs the same NCL plotting scripts in parallel
Climatology Files Created by the AMWG, OMWG, Land and Ice Diagnostic Packages

ATM - SE

ICE

LND
b.e12.B1850C5CN.ne30_g16.init.ch.027.clm2.h0_ANN_ALL.nc  b.e12.B1850C5CN.ne30_g16.init.ch.027.clm2.h0_JJA_climo.nc  b.e12.B1850C5CN.ne30_g16.init.ch.027.clm2.h0_MAM_climo.nc  b.e12.B1850C5CN.ne30_g16.init.ch.027.clm2.h0_SON_climo.nc  b.e12.B1850C5CN.ne30_g16.init.ch.027.clm2.h0_ANotts_climo.nc  b.e12.B1850C5CN.ne30_g16.init.ch.027.clm2.h0_DJF_climo.nc  b.e12.B1850C5CN.ne30_g16.init.ch.027.clm2.h0_MAMS_climo.nc  b.e12.B1850C5CN.ne30_g16.init.ch.027.clm2.h0_JAMS_climo.nc

OCN

57+ Climatology Files are Created
### Climatology Files Created by the AMWG, OMWG, Land and Ice Diagnostic Packages

<table>
<thead>
<tr>
<th>ATM - SE</th>
<th>11 min</th>
</tr>
</thead>
<tbody>
<tr>
<td>ICE</td>
<td>5 min</td>
</tr>
<tr>
<td>LND</td>
<td>18 min</td>
</tr>
<tr>
<td>OCN</td>
<td>8+ hours</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td>8-9 hours</td>
</tr>
</tbody>
</table>

(1 degree resolution climatologies over 10 years)
Climatology Files Created by the AMWG, OMWG, Land and Ice Diagnostic Packages

### ATM-SE

- Original: 11 min
- PyAverager: 48 sec

### ICE

- Original: 5 min
- PyAverager: 11 sec

### LND

- Original: 18 min
- PyAverager: 30 sec

### OCN

- Original: 8+ hours
- PyAverager: 2 min

---

**PyAverager increased performance by x100**

**Total**

- Original: 8-9 hours
- PyAverager: Less than 4 min

(1 degree resolution climatologies over 10 years)
Partitioning of the PyAverager Tasks

Time Averages (Internal Memory)

Time-Series Files

Averages to Compute

InterCommunicator 1

InterCommunicator 2

InterCommunicator 3
New CESM/CMIP6 Workflow

Model Run

- CESM Model Run

Post-Processing

- Time Series Conversion (PyReshaper)
- Re-Designed Diagnostics (PyAverager for climos)

- New Data Compliance Tool

Publication

- Push to ESGF (Improved process)

Automated Task Submission to Machine Queue

Experiments

Update Their Status in Run Database
• This was one of the most expensive CMIP5 post-processing steps
• The current post-processing suite works in serial using NCO
Task Parallelization Strategy
PyReshaper

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

## PyReshaper Timing Statistics

<table>
<thead>
<tr>
<th>Existing Method (NCO)</th>
<th>Time (per MIP per Year)</th>
<th>Average Throughput (per run)</th>
</tr>
</thead>
<tbody>
<tr>
<td>f09 x g16</td>
<td>225 minutes</td>
<td>1.85 MB/sec</td>
</tr>
<tr>
<td>ne120 x g16</td>
<td>478 minutes</td>
<td>4.85 MB/sec</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>
</tr>
</thead>
<tbody>
<tr>
<td>f09 x g16</td>
<td>4 minutes</td>
<td>104 MB/sec</td>
</tr>
<tr>
<td>ne120 x g16</td>
<td>8 minutes</td>
<td>290 MB/sec</td>
</tr>
</tbody>
</table>

- Times include the approximate full time to convert all component data to NetCDF4
- Conversions were ran on Yellowstone using 4 nodes/4 cores (16 cores total)
- We can expect a 2X increase in throughput if we double core counts for low-resolution data
- We can expect a 3X increase in throughput if we double core counts for high-resolution data
New CESM/CMIP6 Workflow

Model Run

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

Publication
- Push to ESGF (Improved process)

Automated Task Submission to Machine Queue

Experiments Update Their Status in Run Database
Data Compliance Tool

• Two Main Goals:
  – Simplify the use
  – Add parallelization to increase performance (this was another bottleneck in CMIP5)

• Use similar techniques that were used by the PyReshaper and PyAverager

• Prototyping work has been started with very promising results
New CESM/CMIP6 Workflow

Model Run

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

Publication
- Push to ESGF (Improved process)

Automated Task Submission to Machine Queue

Experiments Update Their Status in Run Database

CESM Model Run
ESGF Publication

• Move the data staging, directory structuring, and versioning responsibilities into the new compliance tool
• Streamline the submission process
• Test publication workflow for other ways we can improve the publication process
Tool Availability

• PyReshaper
  – https://github.com/NCAR-CISL-ASAP/PyReshaper
  – pip install PyReshaper

• PyAverager
  – https://github.com/NCAR-CISL-ASAP/pyAverager
  – pip install pyAverager

• ASAPPyTools
  – pip install ASAPTools

• Automated Job Launch
  – cesm1_4_beta05/cime1.1.0

• Python Tools Website
  – https://www2.cisl.ucar.edu/tdd/asap/parallel-python-tools-post-processing-climate-data
Questions?

• PyReshaper
  – [https://github.com/NCAR-CISL-ASAP/PyReshaper](https://github.com/NCAR-CISL-ASAP/PyReshaper)
  – pip install PyReshaper

• PyAverager
  – pip install pyAverager

• ASAPPyTools
  – pip install ASAPTools

• Automated Job Launch
  – cesm1_4_beta05/cime1.1.0

• Python Tools Website