Optimizing Workflow for CESM

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- Ben Andre
- Alice Bertini
- John Dennis
- Jim Edwards
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- Michael Levy
- Sheri Mickelson
- Kevin Paul
- Sean Santos
- Jay Shollenberger
- Gary Strand
- Mariana Vertenstein
Current CESM Workflow

Model Run

- CESM Model Run

Post-Processing

- Time Series Conversion (NCO)
- Diagnostics (NCO/NCL)
- CMOR

Publication

- Push to ESGF

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

CESM Model Run

Time Series Conversion (PyReshaper)

Re-Designed Diagnostics (PyAverager for climos)

New Data Compliance Tool

Push to ESGF (Improved process)

Experiments Update Their Status in Run Database

Post-Processing

Publication

Automated Task Submission to Machine Queue
New CESM/CMIP6 Workflow

Model Run

Post-Processing

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

Publication

- New Data Compliance Tool
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Experiments Update Their Status in Run Database

Automated Task Submission to Machine Queue
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
- 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

Automated Task Submission to Machine Queue

Model Run

CESM Model Run

Post-Processing

Time Series Conversion (PyReshaper)

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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 run 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
b.e12.B1850C5CN.ne30_g16.init.ch.027.cam.h0_07_climo.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.cam.h0_01_climo.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.cam.h0_JJA_climo.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.cam.h0_09_climo.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.cam.h0_03_climo.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.cam.h0_JJA_climo.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.cam.h0_11_climo.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.cam.h0_12_climo.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.cam.h0_08_climo.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.cam.h0_04_climo.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.cam.h0_02_climo.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.cam.h0_MAM_climo.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.cam.h0_05_climo.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.cam.h0_06_climo.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.cam.h0_00_climo.nc

ICE
ice_vol_b.e12.B1850C5CN.ne30_g16.init.ch.027.1-10.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.cice.h_amj_climo.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.cice.h_ANN_climo.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.cice.h_jas_climo.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.cice.h_ond_climo.nc

LND
b.e12.B1850C5CN.ne30_g16.init.ch.027.clim2.h0_1-10.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.clim2.h0_ANN_ALL.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.clim2.h0_JJA_climo.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.clim2.h0_MAM_climo.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.clim2.h0_0001-0010.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.clim2.h0_DJF_means.nc

OCN
Arc_hor_mean_hor.meanConcat.b.e12.B1850C5CN.ne30_g16.init.ch.027.pop.h_0001-0010.nc
Hud_hor_mean_hor.meanConcat.b.e12.B1850C5CN.ne30_g16.init.ch.027.pop.h_0001-0010.nc
Atl_hor_mean_hor.meanConcat.b.e12.B1850C5CN.ne30_g16.init.ch.027.pop.h_0001-0010.nc
Ind_hor_mean_hor.meanConcat.b.e12.B1850C5CN.ne30_g16.init.ch.027.pop.h_0001-0010.nc
Lab_hor_mean_hor.meanConcat.b.e12.B1850C5CN.ne30_g16.init.ch.027.pop.h_0001-0010.nc
Gin_hor_mean_hor.meanConcat.b.e12.B1850C5CN.ne30_g16.init.ch.027.pop.h_0001-0010.nc
Sou_hor_mean_hor.meanConcat.b.e12.B1850C5CN.ne30_g16.init.ch.027.pop.h_0001-0010.nc
Glo_hor_mean_hor.meanConcat.b.e12.B1850C5CN.ne30_g16.init.ch.027.pop.h_0001-0010.nc
Pac_hor_mean_hor.meanConcat.b.e12.B1850C5CN.ne30_g16.init.ch.027.pop.h_0001-0010.nc

57+ Climatology Files are Created
<table>
<thead>
<tr>
<th>Package</th>
<th>Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>ATM-SE</td>
<td>11 min</td>
</tr>
<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>
</tbody>
</table>

**Total**: 8-9 hours (1 degree resolution climatologies over 10 years)
## Climatology Files Created by the AMWG, OMWG, Land and Ice Diagnostic Packages

<table>
<thead>
<tr>
<th></th>
<th>Original</th>
<th>PyAverager</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>ATM-SE</strong></td>
<td>11 min</td>
<td>48 sec</td>
</tr>
<tr>
<td><strong>ICE</strong></td>
<td>5 min</td>
<td>11 sec</td>
</tr>
<tr>
<td><strong>LND</strong></td>
<td>18 min</td>
<td>30 sec</td>
</tr>
<tr>
<td><strong>OCN</strong></td>
<td>8+ hours</td>
<td>2 min</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td>8-9 hours</td>
<td>Less than 4min</td>
</tr>
</tbody>
</table>

(1 degree resolution climatologies over 10 years)

**PyAverager increased performance by x100**
Partitioning of the PyAverager Tasks

Averages to Compute:
- AVG 1
- AVG 2
- AVG 3
- AVG 4
- AVG 5
- AVG 6
- AVG 7
- AVG 8
- AVG 9

Time-Series Files:
- Var 1
- Var 2
- Var 3

Time Averages (Internal Memory):
- Rank 1
- Rank 2
- Rank 3

Time Averaged Climatology File:
- Avg Var 1
- Avg Var 2
- Avg Var 3

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
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- Re-Designed Diagnostics (PyAverager for climos)
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- Push to ESGF (Improved process)

Experiments Update Their Status in Run Database

Automated Task Submission to Machine Queue
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
  - CESM Model Run
  - Time Series Conversion (PyReshaper)
  - Re-Designed Diagnostics (PyAverager for climos)
  - New Data Compliance Tool
  - New CESM/CMIP6 Workflow

- Post-Processing
  - Automated Task Submission to Machine Queue
  - Push to ESGF (Improved process)

- Publication
  - Experiments Update Their Status in Run Database
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](https://github.com/NCAR-CISL-ASAP/PyReshaper)
  - `pip install PyReshaper`

- **PyAverager**
  - [https://github.com/NCAR-CISL-ASAP/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](https://www2.cisl.ucar.edu/tdd/asap/parallel-python-tools-post-processing-climate-data)
Questions?

• 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

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