Optimizing Workflow for CESM

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Thanks to all of the CESM workflow refactor team for their work and guidance

• Ben Andre
• Alice Bertini
• John Dennis
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• Sheri Mickelson
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• Gary Strand
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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

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

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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
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Automated Task Submission to Machine Queue
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
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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_SON_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_DJF_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_MAM_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_05_climo.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.cam.h0_10_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_06_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_08_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_02_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_10_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_06_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_jas_climo.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.cice.h_ond_climo.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.cice.h_jfm_climo.nc

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_means.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.clm2.h0_MAM_means.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.clm2.h0_SON_means.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.clm2.h0_DJF_means.nc
b.e12.B1850C5CN.ne30_g16.init.ch.027.clm2.h0_MONS_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
# Climatology Files Created by the AMWG, OMWG, Land and Ice Diagnostic Packages

<table>
<thead>
<tr>
<th>ATM-SE</th>
<th>ICE</th>
<th>LND</th>
<th>OCN</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>11 min</td>
<td>5 min</td>
<td>18 min</td>
<td>8+ hours</td>
<td>8-9 hours (1 degree resolution climatologies over 10 years)</td>
</tr>
</tbody>
</table>
### 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>ATM-SE</td>
<td>11 min</td>
<td>48 sec</td>
</tr>
<tr>
<td>ICE</td>
<td>5 min</td>
<td>11 sec</td>
</tr>
<tr>
<td>LND</td>
<td>18 min</td>
<td>30 sec</td>
</tr>
<tr>
<td>OCN</td>
<td>8+ hours</td>
<td>2 min</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>8-9 hours</td>
<td>Less than 4min</td>
</tr>
</tbody>
</table>

**PyAverager increased performance by x100**

(1 degree resolution climatologies over 10 years)
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 0
- Rank 1
- Rank 2
- Rank 3

InterCommunicator 1

InterCommunicator 2

InterCommunicator 3
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Automated Task Submission to Machine Queue
• 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

Slice 1
Field 1
Field 2
Field 3

Slice 2
Field 1
Field 2
Field 3

Slice 3
Field 1
Field 2
Field 3

Series 1
Field 1

Series 2
Field 2

Series 3
Field 3

Rank 1

Rank 2

Rank 3
### 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.
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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

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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](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