Light-Weight Parallel Python Tools for Earth System Modeling Workflows

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The Problem
Big Data in Earth System Modeling

- NCAR’s Community Earth System Model:
  - Massively parallel (MPI-based)
  - Higher resolution simulations
    - ... “Big Data”!

- Coupled Model Intercomparison Project:
  - CMIP5 (2010-2013):
    - 20 different institutions from around the world!
    - CESM: 2.5 PB generated ➔ 175 TB published
    - Ran out of time before completing publication!
  - CMIP6 (2016-2020):
    - EXPECT: 12 PB generated ➔ 6 PB published
Post-Processing: Why so slow?

- All post-processing steps are serial scripts
  - **Parallelize**
- Required human intervention between steps
  - **Automate**
- Error prone workflow
  - **Thorough testing**
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Light-Weight Parallel Python Tools for ESM
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Approach & Design
Principle of Least Astonishment

- Don’t change anything that already works!
  - Existing workflow is fine for “little data”
- “Minimally Transformative”
  - Fewest changes seen by the user
  - Best way to achieve “buy-in” from users
  - Target & replace the “bottleneck” scripts
- Requires the least development
  - Fastest to solution
  - Easiest to maintain
- Biggest “bang for the buck”
Why Python?

- Rapid prototyping
- CESM Workflow is already script-driven
- Easily extensible
- Modular
- Existing Module Functionality:
  - `numpy`
    - fast array-based data manipulation
  - `mpi4py`
    - Fits into CESM MPI-based workflow
    - No new knowledge to run on supercomputers
  - `PyNIO`
    - NCAR’s multi-format (netCDF, grib, etc) I/O library
Testing
Testing Datasets

<table>
<thead>
<tr>
<th>Component Model Name</th>
<th>Resolution</th>
<th>Total Size (GB)</th>
<th>Number of Time-Series Variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ice</td>
<td>1 degree</td>
<td>8.2</td>
<td>117</td>
</tr>
<tr>
<td></td>
<td>0.1 degree</td>
<td>556</td>
<td>112</td>
</tr>
<tr>
<td>Ocean</td>
<td>1 degree</td>
<td>190</td>
<td>114</td>
</tr>
<tr>
<td></td>
<td>0.1 degree</td>
<td>3100</td>
<td>34</td>
</tr>
<tr>
<td>Atmosphere</td>
<td>1 degree</td>
<td>30</td>
<td>132</td>
</tr>
<tr>
<td></td>
<td>¼ degree</td>
<td>1000</td>
<td>198</td>
</tr>
<tr>
<td>Land</td>
<td>1 degree</td>
<td>8.7</td>
<td>297</td>
</tr>
<tr>
<td></td>
<td>¼ degree</td>
<td>88</td>
<td>150</td>
</tr>
</tbody>
</table>

- Datasets span 10 years of monthly data
Testing Platform

- NCAR’s Yellowstone, GLADE & GPFS:
  - ~90 GB/s peak from GPFS
  - ~1.5 GB/s from each compute node
The PyReshaper: “Time-Series Generation”
Time Slices (Raw Format)

Slice 1
Field 1
Field 2
Field 3

Slice 2
Field 1
Field 2
Field 3

Slice 3
Field 1
Field 2
Field 3

Slice 4
Field 1
Field 2
Field 3

Slice 5
Field 1
Field 2
Field 3

Time Series (Archive Format)

Series 1
Field 1
Field 2
Field 3

Series 2
Field 1
Field 2
Field 3

Series 3
Field 1
Field 2
Field 3

Time
Task Parallelism

Light-Weight Parallel Python Tools for ESM

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- Run with 4 nodes / 4 processors per node
  - Greater parallelism available!
- Overall 12x speedup ("sum of all times")
  - 7x for Low-Resolution / 14x for High-Resolution
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The PyAverager: “Climatology Computation”
Time Slices (Raw Format)

Slice 1
- Field 1
- Field 2
- Field 3

Slice 2
- Field 1
- Field 2
- Field 3

Slice 3
- Field 1
- Field 2
- Field 3

Climatology (Time Averages)

Climatology 1
- Field 1
- Field 2
- Field 3

TO
Time Series (Archive Format)

Series 1
Field 1
Series 2
Field 2
Series 3
Field 3

Time

Climatology (Time Averages)

Climatology 1
Field 1
Field 2
Field 3

TO

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Time Slices (Raw Format)

- Slice 1
  - Field 1
  - Field 2
  - Field 3
- Slice 2
  - Field 1
  - Field 2
  - Field 3
- Slice 3
  - Field 1
  - Field 2
  - Field 3

Climatology (Time Averages)

- Climatology 1
  - Field 1
  - Field 2
  - Field 3

To
Task Parallelism

Time Averages computed in Rank memory

Air • Planet • People

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Task Parallelism

Time Averages computed in Rank memory
Task Parallelism

- Additional Parallelism over Climatologies
  - Seasons
  - Years
  - Months
- Climatologies Ordered:
  - Mos ➔ Seasons ➔ Yrs
- Each Climatology given its own MPI subcommunicator

Light-Weight Parallel Python Tools for ESM
- Incredible!
  - Overall 136x speedup!
  - 130x for Low-Resolution / 138x for High-Resolution
- Overall 27x speedup ("sum of all times")
  - 6x for Low-Resolution / 32x for High-Resolution
- Overall 27x speedup ("sum of all times")
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Conclusions & Future Work
Done!

- Began a new development program:
  - Minimally transformation / Maximal benefit
  - “Principle of Least Astonishment”

- New tools:
  - PyReshaper (Overall 12x Speedup)
  - PyAverager (Overall 27x Speedup)
  - Common Dependency: ASAP Python Toolbox
  - Available on GitHub:
    - [https://github.com/NCAR-CISL-ASAP/](https://github.com/NCAR-CISL-ASAP/)
Yet to be done...

- Data Parallelism
  - Python-based NetCDF Parallel Write
  - Should improve scalability of tools
- New Parallel Publication Preparation Tool
  - CMIP Formatting Conversion (“CMOR”)
  - In development
Thanks!

Thanks to the NSF, and special thanks to NCAR’s CESM Development Team for all there help with testing and design.