A new workflow for CESM™ to address CMIP6 challenges

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3rd ENES Workshop on Workflows
13 September 2018
The Community Earth System Model (CESM)

- CESM is a fully-coupled climate model
- CESM is sponsored by the National Science Foundation and the U.S. Department of Energy, with contributions from the University community

Image credit: https://www2.cisl.ucar.edu/software/community-models

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Lessons We Learned From CMIP5

- CESM was the first model to complete their simulations, but the last to complete publication. Why?
  - All of the post-processing was serial and it took a long time to run
  - Workflow was error prone and was time consuming to debug
  - Too much human intervention was needed between post-processing steps and time was wasted
  - There was only one person who knew the status of all of the experiments
NCAR’s CMIP6 Plans
(DECK and Tier I Experiments)

• Currently participating in about 23 MIPS
  – Just over 100 different experiments total

• Over all experiments, we will simulate roughly 23,287 years of climate

• The total cost will be roughly 230M core hours

Complexity Comparison

CMIP5
- 25 Experiments
- Timeline: 3 years
- Output size: 800TB
- Published size: 200TB

CMIP6
- 102 Experiments
- Timeline: 1 year
- Output size: 8PB (estimate)
- Published size: 2PB (estimate)
Complexity Comparison

**CMIP5**
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We needed better methods!
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New CESM/CMIP6 Workflow

Model Run

- CESM Model Run

Post-Processing

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

Publication

- Push to ESGF

Automated Workflow Using Cylc

Increased Performance

- Wrote new versions of these tools in Python and added parallelization
- Experiments Update Their Status in Run Database
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PyReshaper
Converting files that have all variables and one time step to files that have one variable and multiple time steps

![Average Speedup Among the Simulations (Parallel/Serial)](chart.png)

- Maximum throughput in one day was 25TB
- There was a 13x speedup for monthly output
- There was an overall speedup of 6.5x across all output streams

Timing results credit: Gary Strand

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The climatology files are calculated in parallel and the NCL plotting scripts are ran in parallel.
PyConform - 1st Step
(Python Climate Output Formatter)

• Users need to create a text file with a “definition” that describe input variable(s) to output variable
  – Examples:
    • cfc11global=f11vmr
    • cfc12global=f12vmr
    • ch4=vinth2p(CH4, hyam, hybm, plev19, PS, P0)
    • mc=CMFMC+CMFMCMDZM

• Then users run an input generator script that matches the “definitions” to its variable information within the CMIP6 Data Request
  – The Data Request lists variables requirements:
    • Units
    • Dimensions
    • Descriptions
    • And a lot more ...
Example Input File (json format)

```
"ua": {
    "attributes": {
        ".FillValue": "1e+20",
        "cell_measures": "area: areacella",
        "cell_methods": "time: mean",
        "comment": "Eastward\" indicates a vector component which is positive when directed eastward (negative westward). Wind is defined as a two-dimensional (horizontal) air velocity vector, with no vertical component. (Vertical motion in the atmosphere has the standard name upward_air_velocity.)",
        "description": "Eastward\" indicates a vector component which is positive when directed eastward (negative westward). Wind is defined as a two-dimensional (horizontal) air velocity vector, with no vertical component. (Vertical motion in the atmosphere has the standard name upward_air_velocity.)",
        "frequency": "mon",
        "id": "ua",
        "long_name": "Eastward Wind",
        "mipTable": "Amon",
        "out_name": "ua",
        "prov": "Amon ((isd.003))",
        "realm": "atmos",
        "standard_name": "eastward_wind",
        "time": "time",
        "time_label": "time-mean",
        "time_title": "Temporal mean",
        "title": "Eastward Wind",
        "type": "real",
        "units": "m s-1",
        "variable_id": "ua"
    },
    "datatype": "real",
    "definition": "vinth2p(U,hyam, hybm, plev19, PS, P0)"
}
```

This is just a sample of one of the variable sections. There are other parts of the file that list other variables and then global attributes to be added to the output file.
PyConform - 2\textsuperscript{nd} Step

(Python Climate Output Formatter)

16x to 38x speedup over our old Fortran code and CMOR

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New CESM/CMIP6 Workflow

Automated Workflow Using CyC

Model Run

CESM Model Run

Post-Processing

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Project Management

Each experiment updates its progress automatically in the web based database as it’s running

Experiments Update Their Status in Run Database
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This web based database has been very helpful for managers to check simulation progress and to look at results all in one place.
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New CESM/CMIP6 Workflow

Model Run

- CESM Model Run
- Time Series Conversion (PyReshaper)
- New Data Compliance Tool (PyConform)
- Re-Designed Diagnostics (PyAverager)

Post-Processing

- Automated Workflow Using Cylc
- We’re using Cylc to coordinate the synchronization of all of the workflow tasks in order to reduce human intervention in between tasks

Publication

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Experiments Update Their Status in Run Database
Automatic Suite Generation

**Why?** Because our users are new to Cylc, we wanted to make the transition as easy as possible to help with positive adoption.

**How?** This is possible because CESM and our post-processing tools allow us to query the experiment to get the needed information to set up specific tasks, their dependencies, and how to submit each task to the queue.
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Automatic Suite Generation

Set in the CESM Experiment
XML Files:
- Run Length = 100 yrs
- Restart = Every 10 yrs
- Run diagnostics = Every 10 yrs
- Run timeseries = True
- Conform data = True

The user then runs a script to create the Cytc suite

1. Look at the XML settings in the CESM env
2. Construct a dependency graph based on what the user wants to run and when
3. Look at CESM env to find out how to run each task
4. Create a suite.rc for the user based on this information
5. Register the suite for the user

#!Jinja2
[cyclc]
[scheduling]
[[dependencies]]
  graph = ""
  case_run_0011-01 => case_st_archive_0011-01-01
  case_st_archive_0011-01-01 => case_run_0021-01-01
...
[environment]
[root]
  method = pbs
  execution time limit = PT12H
  execution retry delays = PT30S, PT120S, PT600S
  method = pbs
  execution time limit = PT12H
  execution retry delays = PT30S, PT120S, PT600S
  -q = regular
  -N = b.e21.B1850.f09_g17.CMIP6-piControl.001.run
  -r = n
  -j = oe
  -S = /bin/bash
  -l = select=120:ncpus=36:mpiprocs=12:ompthreads=3
Communication Between Cylc and the Experiment Database

We used a naïve approach of just having Cylc email the database with progress updates and we parse the emails to update the correct database entries.

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Cylc Task

Experiment name

Cylic Event Email

Subject: !!cylc alert!! suite b.e21.BW1850.f09_g17.CMIP6-piControl.001.suite.cmip6 succeeded

-------------

SUITE: b.e21.BW1850.f09_g17.CMIP6-piControl.001.suite.cmip6
MESSAGE: case_run_0151-01-01.1

Status

Simulation Progress

CESM Exp DB

Exp List:
b.e21.BW1850.f09_g17.CMIP6-piControl.001

---

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Simple Workflows

Example of a single member simulation for our piControl CMIP6 experiment

- Simulates 1,000 years of climate under 1850 conditions, with each CESM run task simulating 10 years of climate
- Runs the model and archiving step about 100 times each
- Runs each of the diagnostic packages 10 different times during the simulation, every 100 years
- Creates the timeseries files
- Conforms data to meet CMIP6 standards

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Ensemble Workflows

Example of a 3 member ensemble of our high top historical experiment

Each member:

• Simulates the climate from year 1850 through 2014, each CESM run task simulates 2 years of climate
• Runs the model and archiving step about 82 times each
• Runs each of the diagnostic packages 5 different times during the simulation
• Creates the timeseries files
• Conforms data to meet CMIP6 standards
Other CESM Experiments That Used Cylc (non CMIP6)

- Used Cylc to complete 1,240 out of 1,860 total runs and postprocessed ~750 TB timeslice output in about 1 month

- Used Cylc to run and postprocess part of a 30 member ensemble in a couple of months

- Used Cylc to build and run over 20,000 forecast ensembles in a couple of months
Questions?

- PyReshaper
  - https://github.com/NCAR/pyreshaper

- PyAverager
  - https://github.com/NCAR/pyAverager

- PyConform
  - https://github.com/NCAR/PyConform

- CESM/Cylc WF
  - https://github.com/NCAR/CESM-WF

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