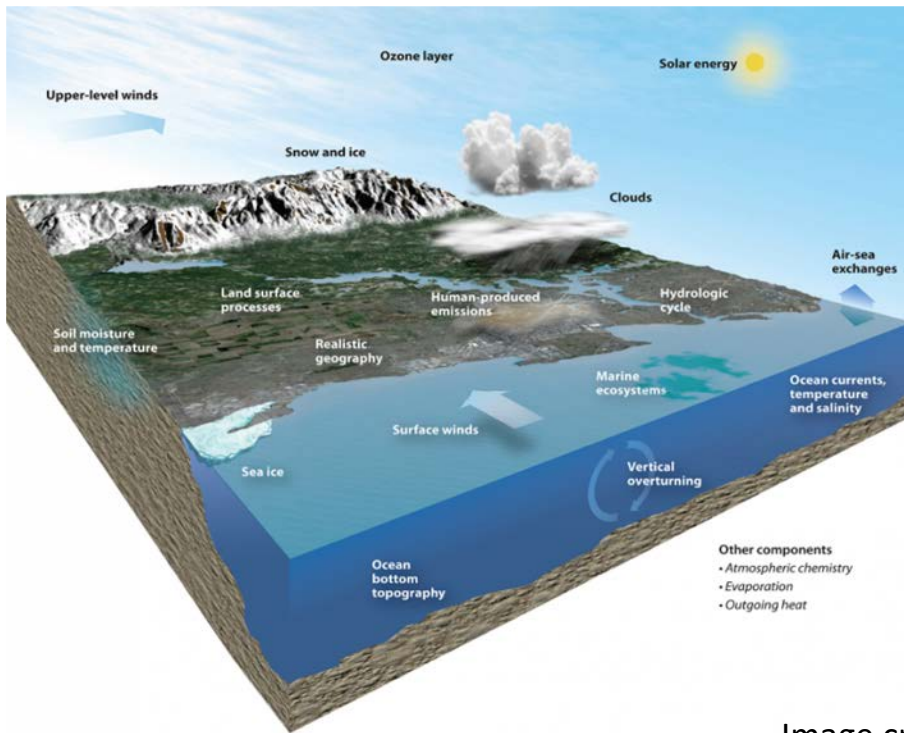


A new workflow for CESM™ to address CMIP6 challenges

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NCAR

3rd ENES Workshop on Workflows
13 September 2018

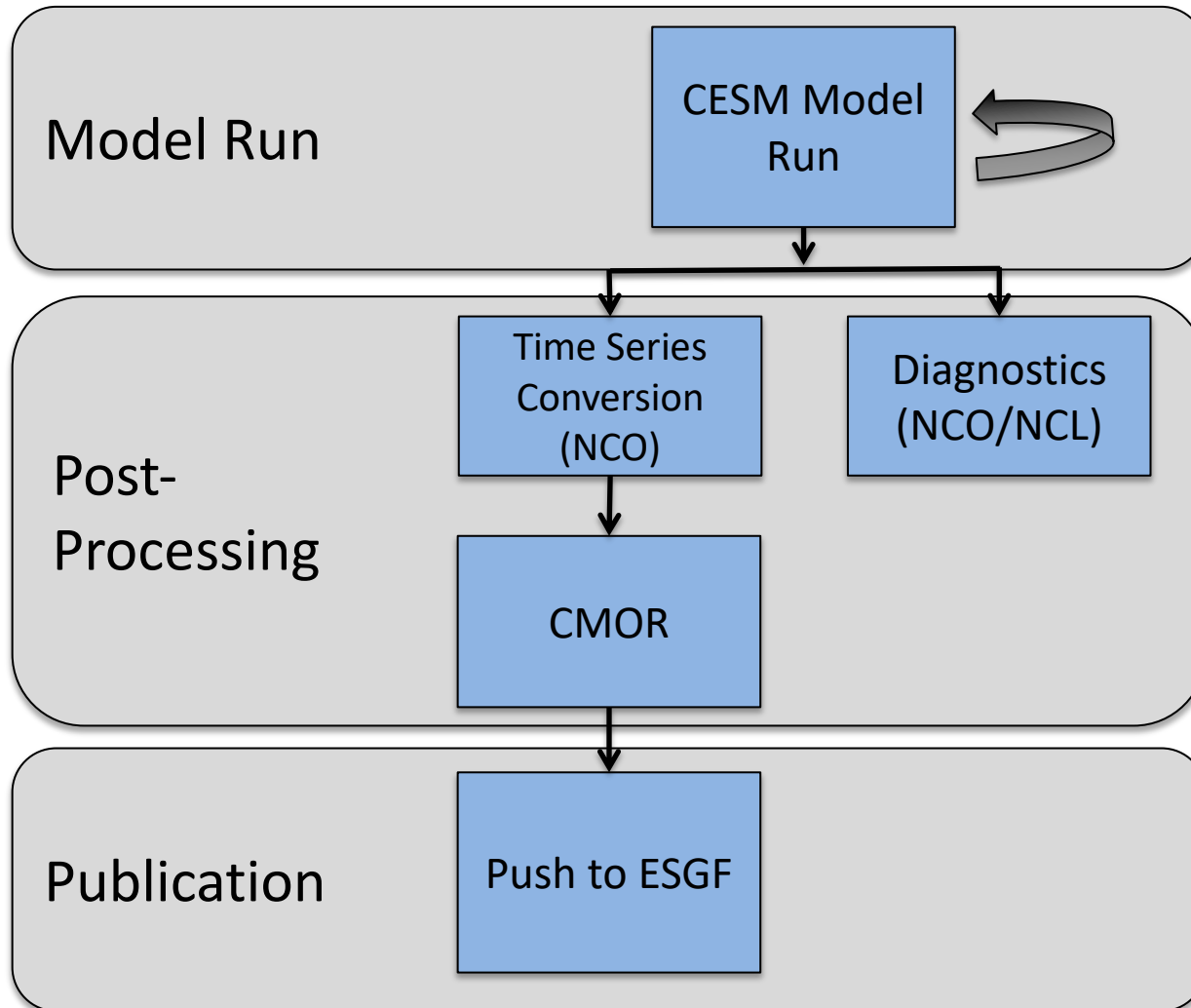
The Community Earth System Model (CESM)



- 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>

CESM's CMIP5 Workflow



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

Background image: Eyring, Veronika & Bony, Sandrine & Meehl, Gerald & A. Senior, Catherine & Stevens, Bjorn & Ronald, Stouffer & E. Taylor, Karl. (2016). Overview of the Coupled Model Intercomparison Project Phase 6 (CMIP6) experimental design and organization. Geoscientific Model Development. 9. 1937-1958. 10.5194/gmd-9-1937-2016.

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

- 25 Experiments
- Timeline: 3 years
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CMIP6

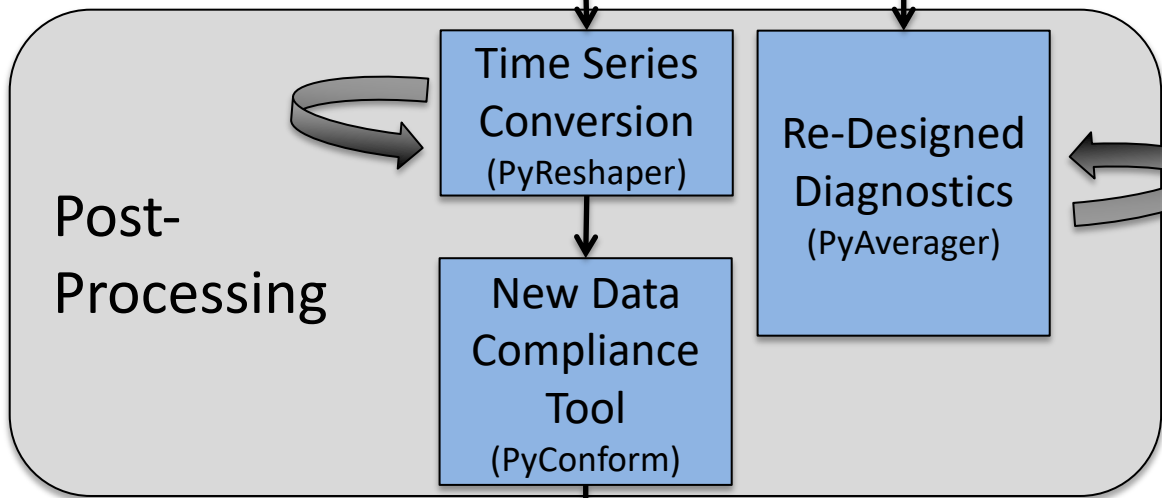
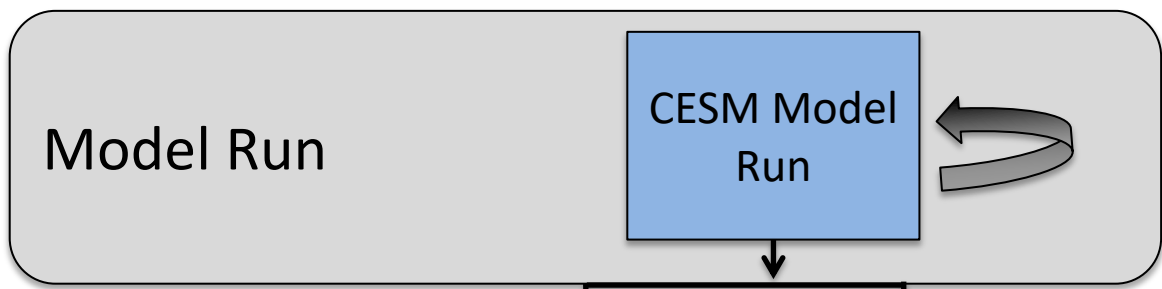
- 102 Experiments
- Timeline: 1 year
- Output size: 8PB (estimate)
- Published size: 2PB (estimate)

We needed better methods!

<http://www.bbc.com/earth/story/20170510-terrifying-20m-tall-rogue-waves-are-actually-real>

New CESM/CMIP6 Workflow

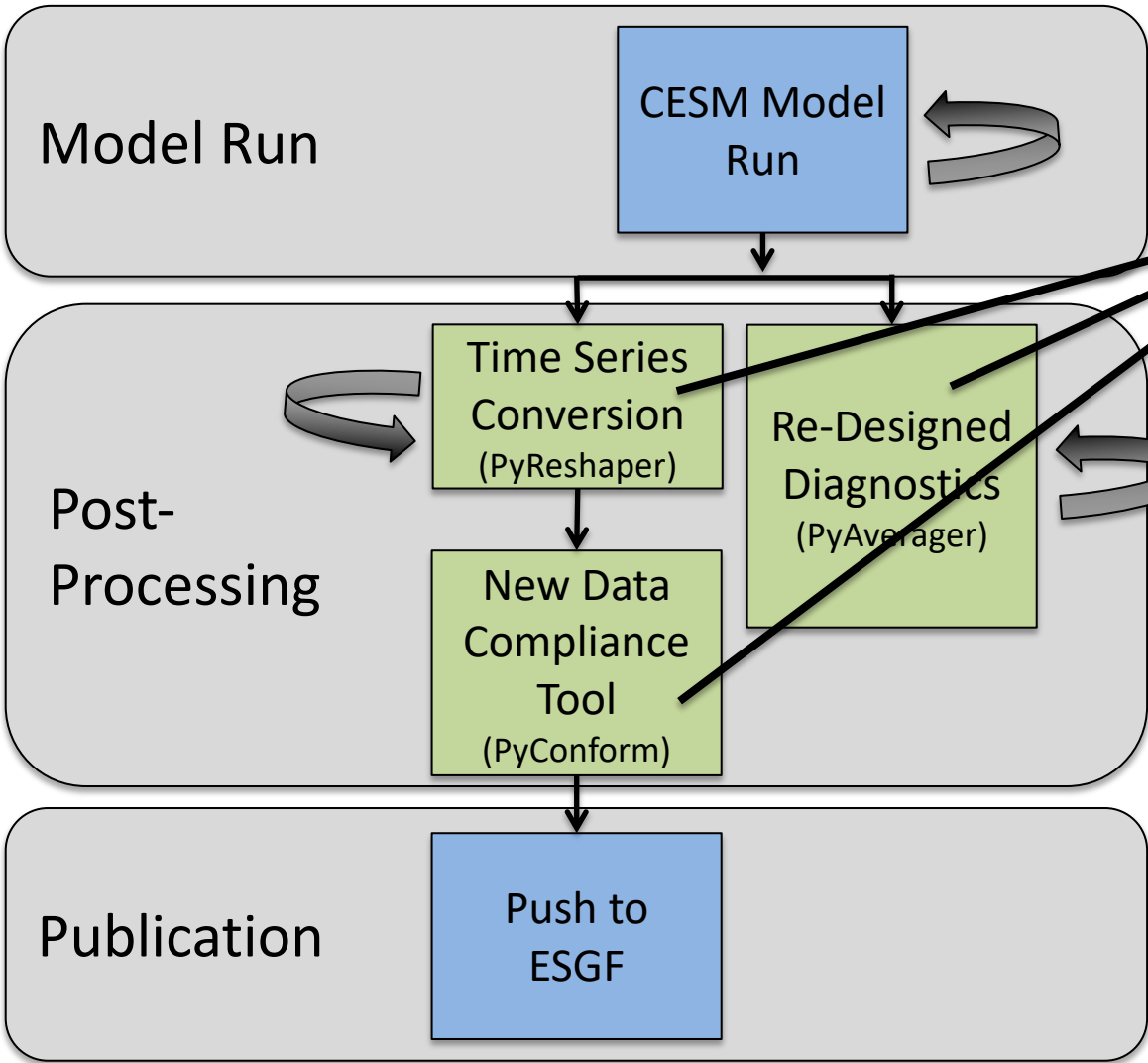
Automated Workflow Using Cylc



Experiments Update Their Status in Run Database

New CESM/CMIP6 Workflow

Automated Workflow Using Cylc

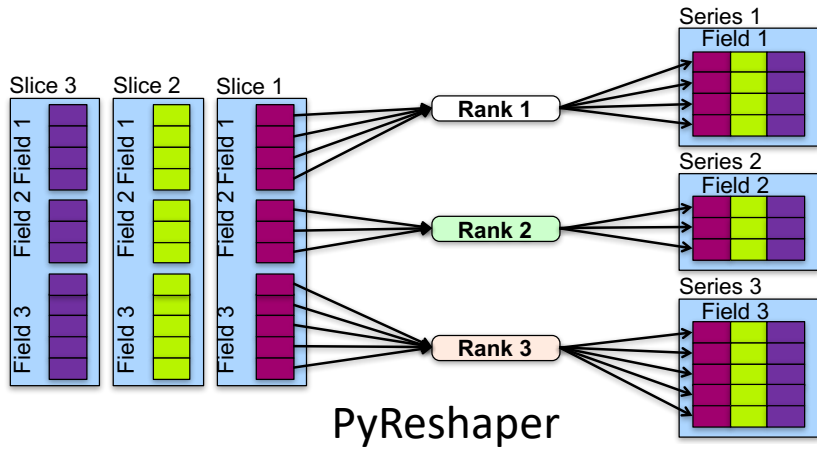


Increased Performance

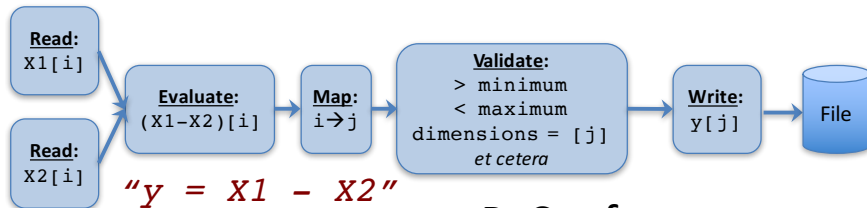
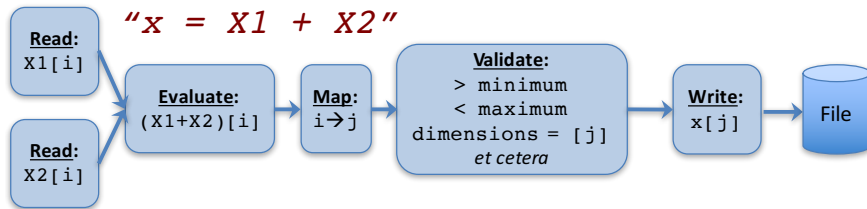
Wrote new versions of these tools in Python and added parallelization

Experiments Update Their Status in Run Database

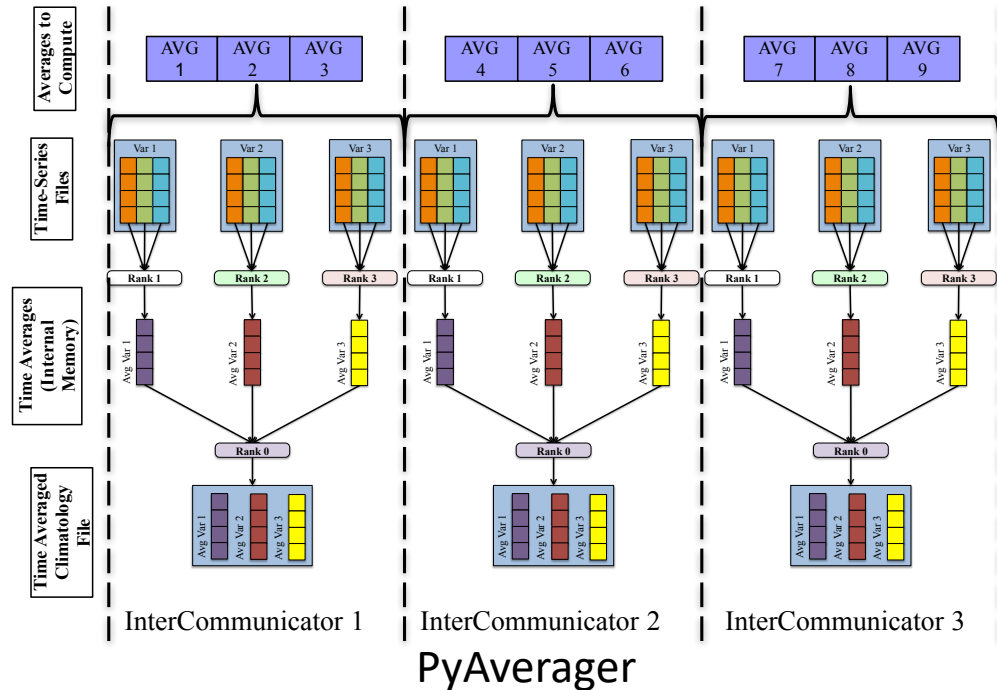
Parallelization Methods



PyReshaper



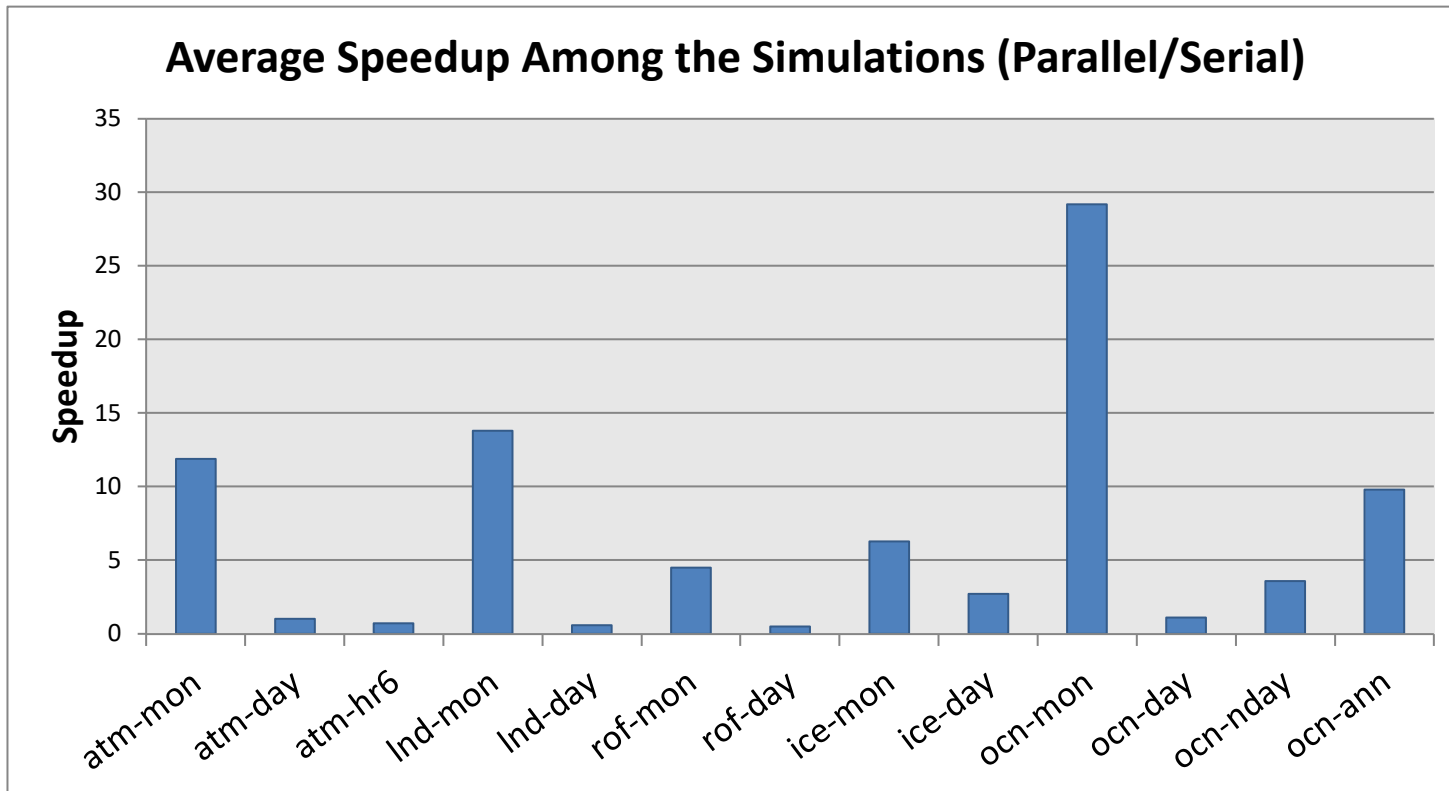
PyConform



PyAverager

PyReshaper

Converts files that have all variables and one time step to files that have one variable and multiple time steps



Timing results credit: Gary Strand

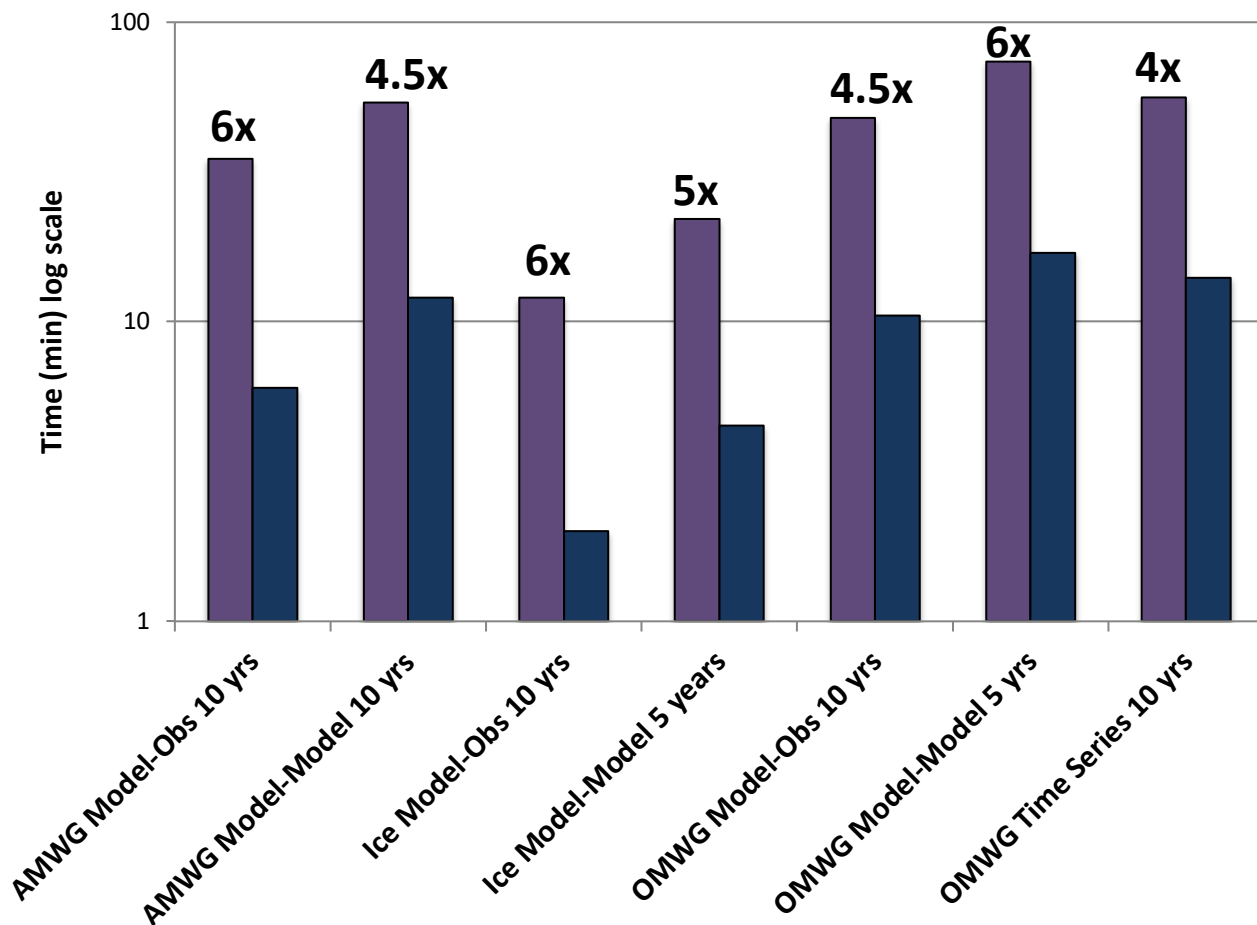
Maximum throughput in one day was 25TB

There was a 13x speedup for monthly output

There was an overall speedup of 6.5x across all output streams

Diagnostic Package Performance Improvements

Performance Comparison Across Diagnostic Packages



The climatology files are calculated in parallel and the NCL plotting scripts are ran in parallel

■ Original
■ PyAverager/NCL 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+CMFMCDZM`
- 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 ...

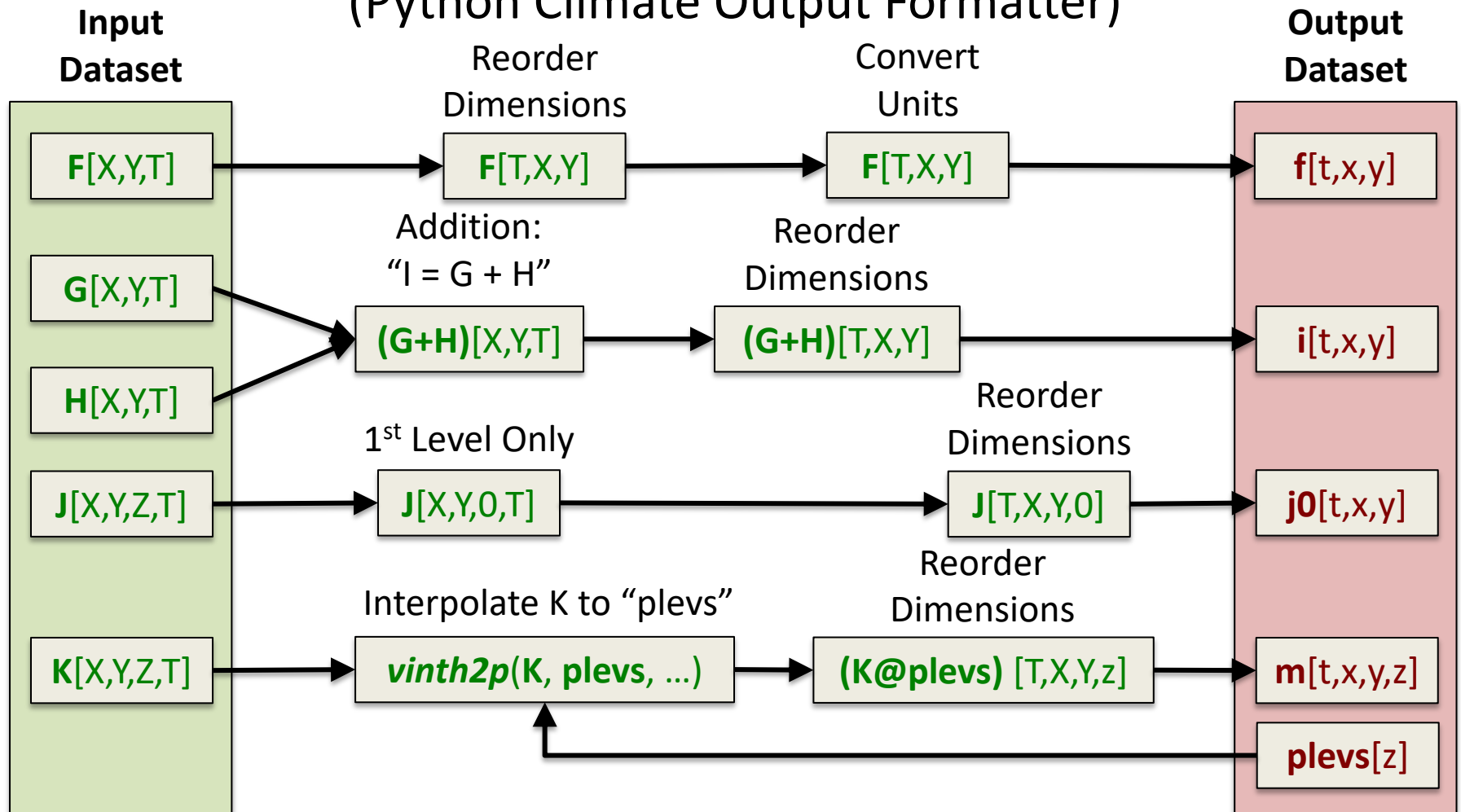
Example Input File (json format)

```
"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 - 2nd Step

(Python Climate Output Formatter)

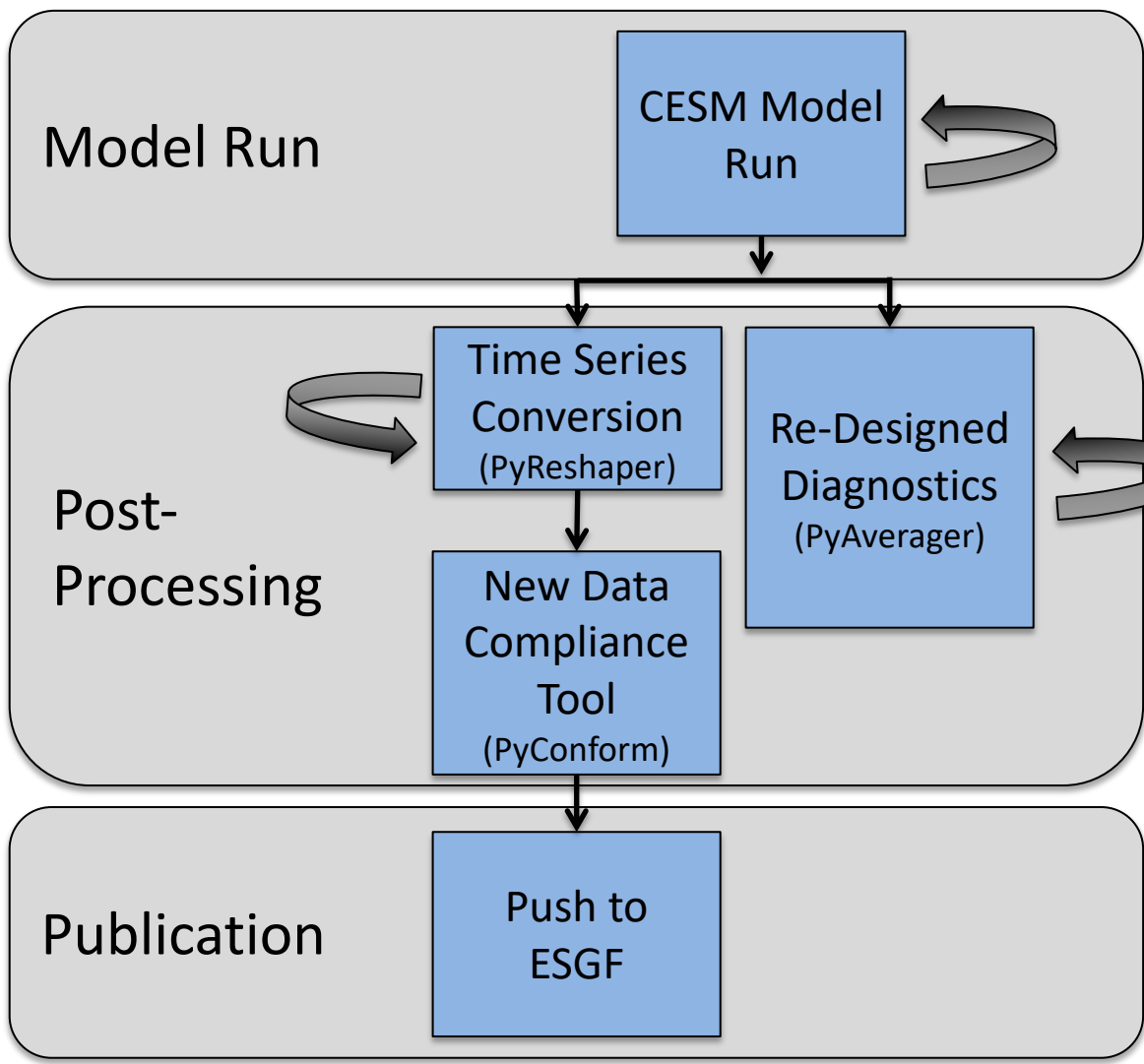


16x to 38x speedup over our old Fortran code and CMOR

Credit: Kevin Paul

New CESM/CMIP6 Workflow

Automated Workflow Using Cylc



Project Management

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



CESM's Experiment Database

CESM2 Experiments Database x

Secure | <https://csegweb.cgd.ucar.edu/expdb2.0/cgi-bin/expList.cgi>

CESM1 Experiments | CESM2 Experiments | Advanced Search | Select a Case Name:

Logged in as | Logout | Help

CESM2 / CMIP 6 Experiments | CESM2.0 Release Experiments | CESM2 Production Experiments | CESM2 Project A Experiments (TBD) | CESM2 Project B Experiments (TBD)

DECK Experiments | MIP Experiments | Decadal Prediction Experiments | Experiments by Name | **Reserve a CMIP6 Case Name** | Overall Experiment Status | Overall Experiment Diagnostics

This form must be completed for every CMIP6 experiment prior to running create_newcase. It contains expert knowledge that cannot be retrieved by the caseroot archive_metadata script required by the CMIP6 project. For details, please see the following **CMIP6 Specific References**:

- View CMIP6 Data Request Definitions
- View CMIP6 Global Attributes, DRS, Filenames, Directory Structure, and Controlled Vocabularies (CVs) for details concerning the "ripf" specification.
- CMIP6 github JSON defined experiment ID's and sources

* Indicates a required field.
CMIP6 Global Attributes are enclosed in ().

General Case Information

* Unique Case Name:

* Brief Title/Description:
(variant_info)

Total number of model years to be run:

* Run Type and Start Date (YYYY-MM-DD):
(branch_method) and (branch_time_in_child)

Startup

Branch

Hybrid

Experiment Ensembles

Is this an ensemble experiment? No Yes

If "Yes", enter the number of ensemble members:

... and number of years for each ensemble member:

Note: Ensemble experiments need to only reserve one unique casename corresponding to the first ensemble name of the experiment. For example, "b.e20.dp.hd-1961.20C.1d.001" is the only case name that needs to be entered for the hindcast initialization of the 20th Century run starting at 1961. Subsequent ensemble member casenames will be automatically added to the database with the last numeric extension incremented for each ensemble member as well as the realization number.

CMIP6 Experiment Associations

* CMIP6 Experiment (experiment_id)

* Variant Label "ripf": realization_index: Note: the CESM2 database will automatically assign a realization number for ensemble experiments

realization_index = an integer (>=1) distinguishing among members of an ensemble of simulations that differ only in their initial conditions (e.g., initialized from different points in a control run). Note that if two different simulations were started from the same initial conditions, the same realization number should be used for both simulations. For example if a historical run with "natural forcings" only and another historical run that includes anthropogenic forcings were both executed at the same point in a control run, both should be assigned the

CESM's Experiment Database

The screenshot shows the CESM Experiments Database web interface. The browser address bar displays the URL <https://csegweb.cgd.ucar.edu/expdb2.0/cgi-bin/expList.cgi>. The page has a navigation bar with tabs for "CESM2 / CMIP 6 Experiments", "CESM2.0 Release Experiments", "CESM2 Production Experiments", "CESM2 Project A Experiments (TBD)", and "CESM2 Project B Experiments (TBD)". Below this, there are sub-tabs for "DECK Experiments", "MIP Experiments", "Decadal Prediction Experiments", "Experiments by Name", "Reserve a CMIP6 Case Name", "Overall Experiment Status", and "Overall Experiment Diagnostics".

The main content area shows a list of experiments. The first experiment is selected, and its details are displayed in a table. The details table has five columns: "model run", "st_archive", "timeseries", "conformer", and "overall status". Each column contains a sub-table with various metrics.

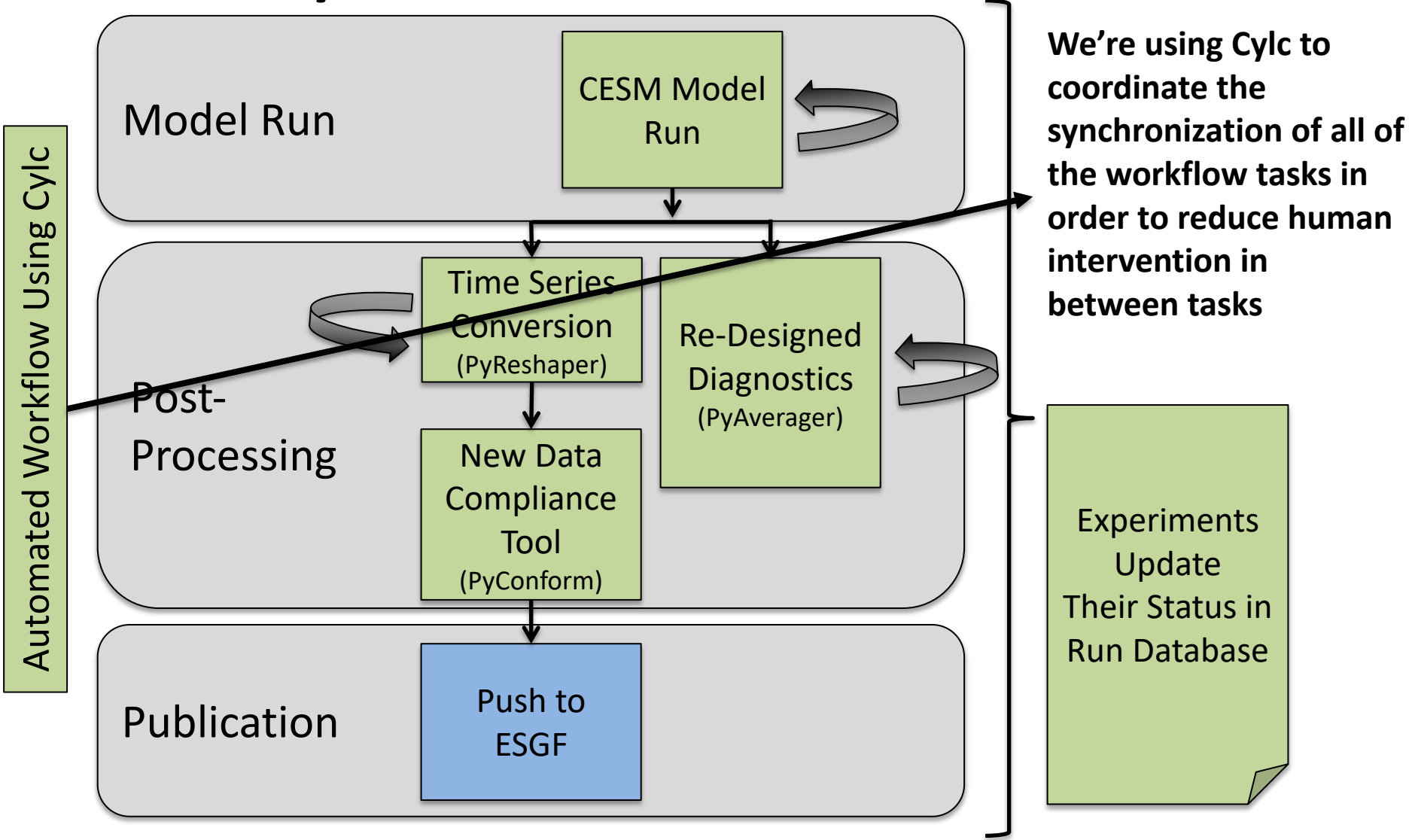
model run	st_archive	timeseries	conformer	overall status
Last Run Date: 0311-01-02	Last Archive Date: 0311-01-01	Last Timeseries Date: 0000-01-01	Last Conform Date: 0000-01-01	Total Disk Usage: 0
Disk Usage: 0	Disk Usage: 0	Disk Usage: 0	Disk Usage: 0	Run Percent Complete: 11%
Cost: undefined	Process Time:	Process Time:	Process Time:	Archive Percent Complete: 11%
Throughput:	Last Update: 2018-08-29 16:07	Last Update: 2018-08-07 13:09	Last Update: 2018-08-07 13:09	Timeseries Percent Complete: -0.1%
Last Update: 2018-08-30 03:06				Conform Percent Complete: -0.1%

Below the details table, there is a list of other experiments, each with a status icon (green plus) and a summary row showing "model run: Started", "st_archive: Succeeded", "timeseries: Unknown", "conformer: Unknown", and "published:".

The bottom of the page shows "Showing 1 to 5 of 5 entries" and navigation buttons for "Previous", "1", and "Next".

This web based database has been very helpful for managers to check simulation progress and to look at results all in one place.

New CESM/CMIP6 Workflow



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

Automatic Suite Generation

User



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
```

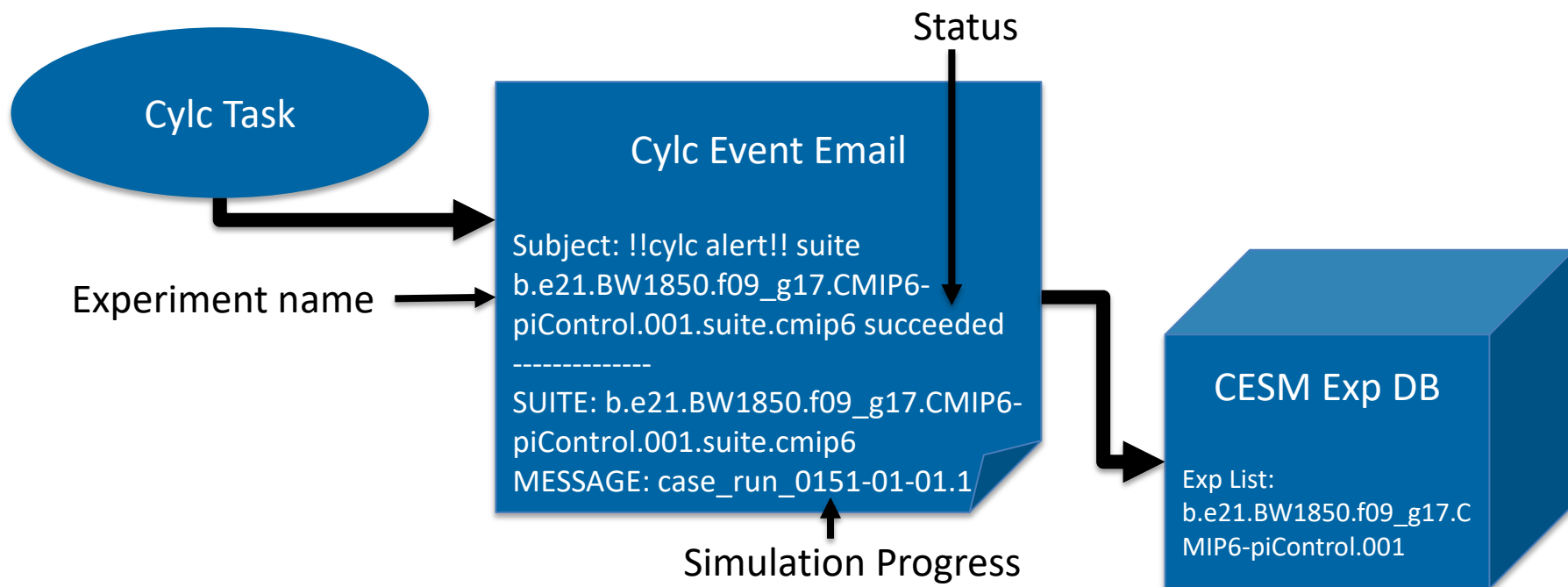
```
#!Jinja2
[cylc]
[scheduling]
  [[dependencies]]
    graph = ""
    case_run_0011-01-01 => case_st_archive_0011-01-01
    case_st_archive_0011-01-01 => case_run_0021-01-01
  ...
[runtime]
  [[root]]
    [[environment]]
      {% for i in range(0,dates_case_run|length) %}
        [[case_run_{{dates_case_run[i]}} ]]
      [[job]]
        method = pbs
        execution time limit = PT12H
        execution retry delays = PT30S, PT120S, PT600S
      [[[directives]]]
        -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
    ...
```

The user then runs a script to create the Cylc 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

Communication Between Cylc and the Experiment Database

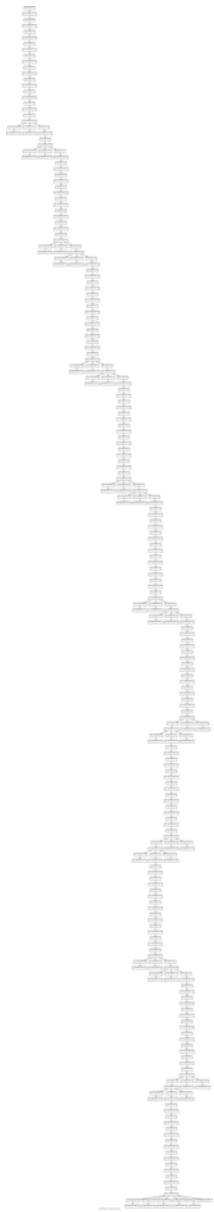
We used a naïve approach of just having Cylc email the database with progress updates and we parse the emails to update the correct database entries



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

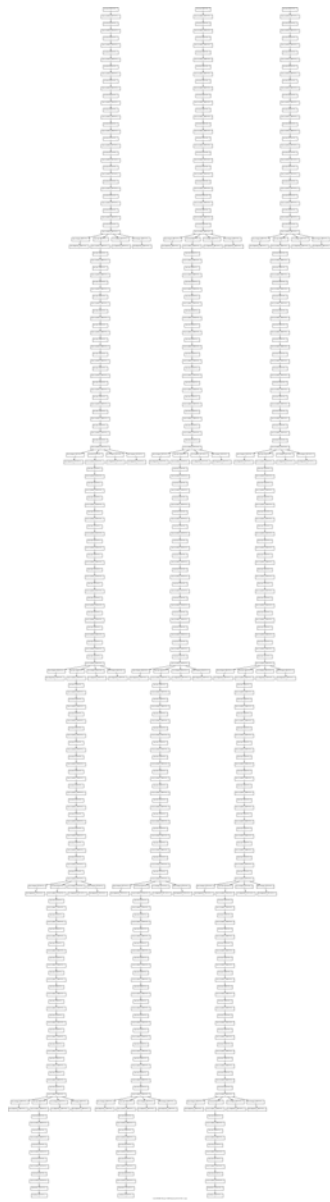


Ensemble Workflows

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>

Contact Info mickelso .at. ucar.edu