# CESM Workflow Refactor Project
# LIMWG and PCWG 2015 Winter Meetings


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CSEG & ASAP/CISL

# CESM Workflow Refactor Project

Who's involved? Joint project between CSEG, CISL and CCP

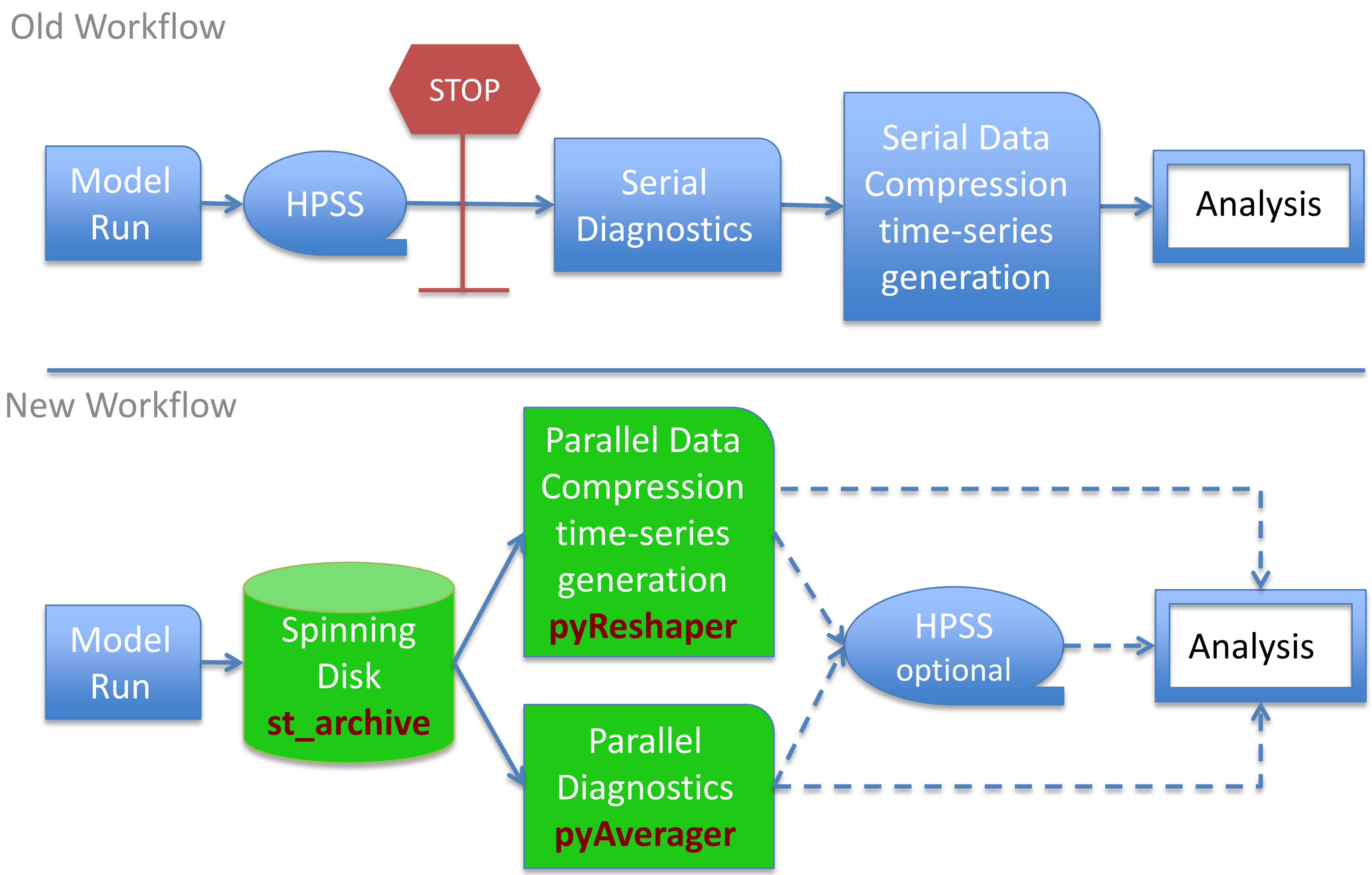
Goals? To create a new end to end workflow that enables scientists to get work done easier and faster

What we're looking to improve? Input data creation, archiving, model variable time-series generation, and post-processing

What is our process? Looking at current workflow functionality and performance and incrementally adding improvements that yield the most "bang for the buck"

# CESM Workflow Refactor Project

Uses NCL, Matlib, XML, Python, and CESM scripts



# CESM Script Modifications

## Problems:

- The current CESM framework can not automate the time-series generation or diagnostic submission
- Existing framework is not flexible and wastes compute cycles

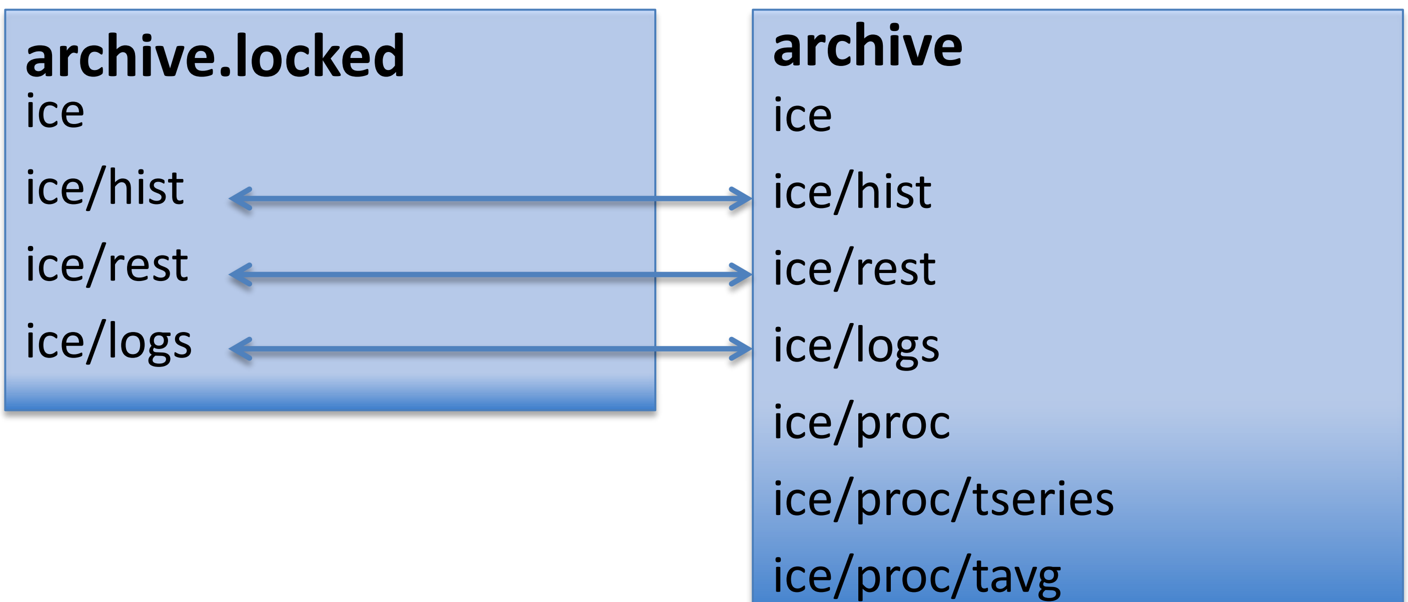
## Solution:

- Automate post-processing tasks submitted as separate dependent jobs in the model run script
- Allow for the flexibility to submit these jobs with different node counts
- Refactor the short-term archive script to create a post-processing location on disk to allow for concurrent model run and post-processing tasks

# Short-Term Archiver

## What it does:

- At model run completion, copies or moves all files from the run directory into the archive directories on disk
- Retains a complete set of restart files in the run directory allowing for a new run job submission
- Controlled by XML
- Follows the CESM output file naming conventions



# Data Compression and Time-Series Generation

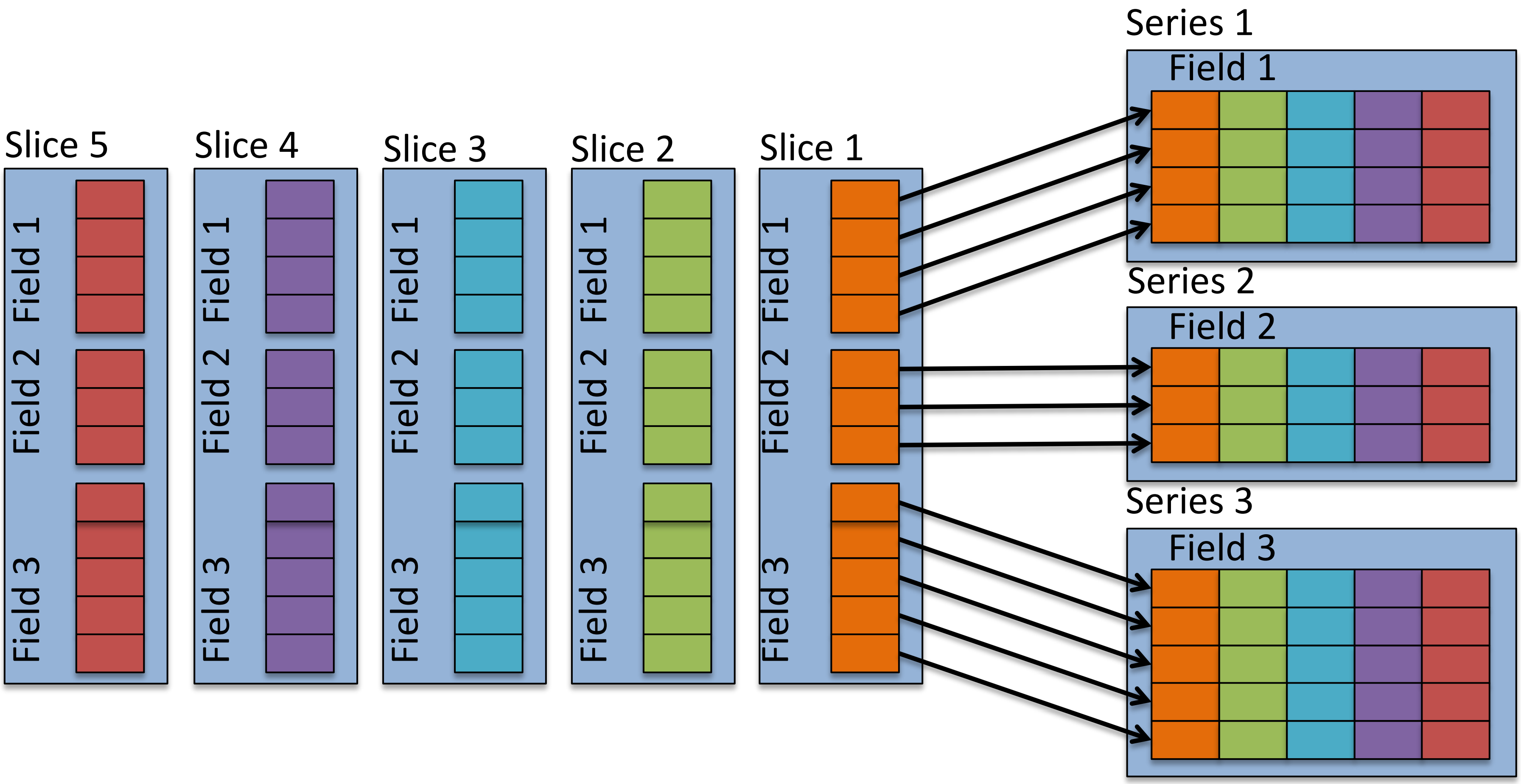
Problems:

- The current post-processing suite works in serial using NCO
- **CMIP5 post-processing required about as much wall-clock time to post-process data as actual model run time**

Solution:

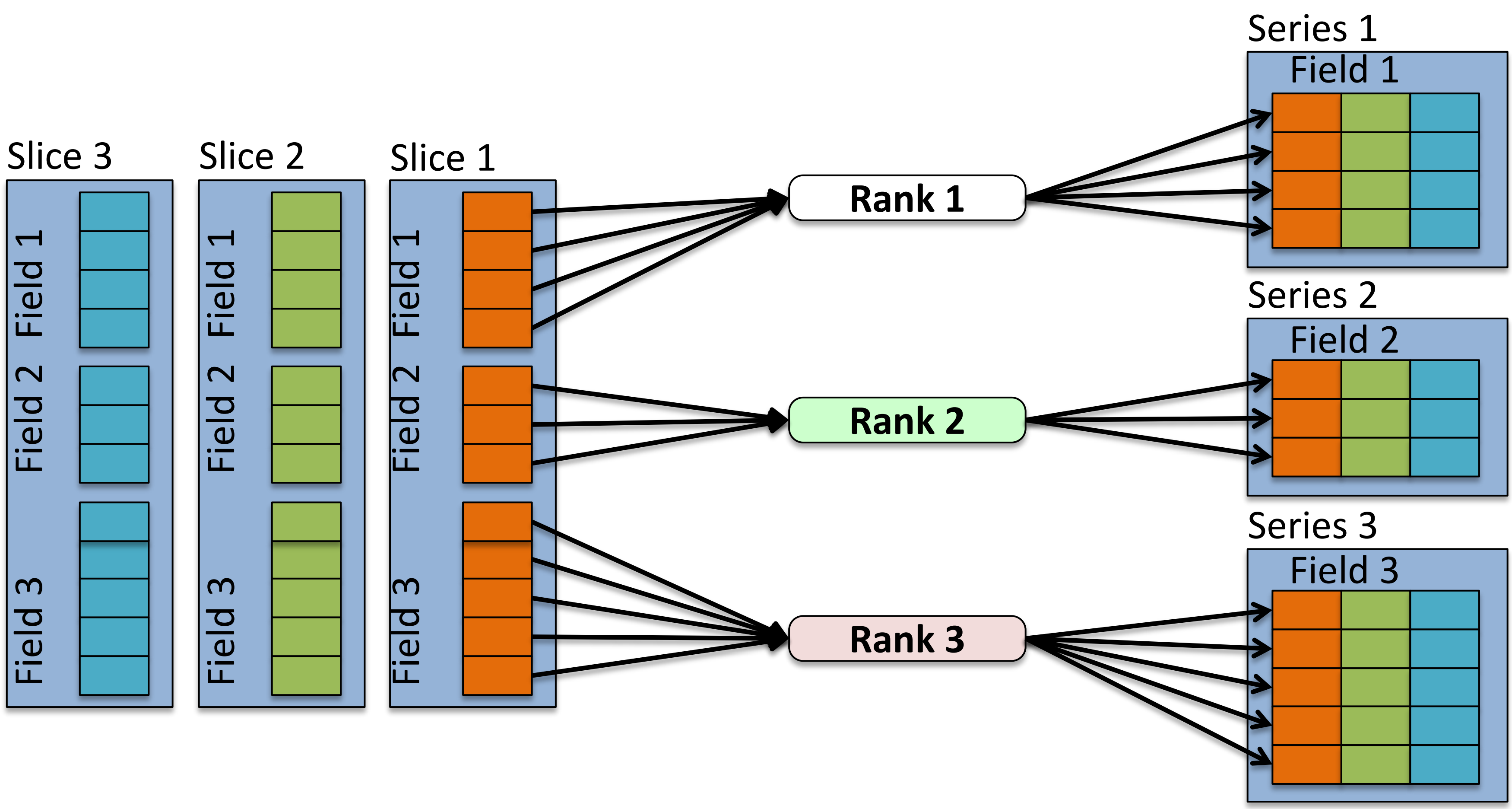
- Light-weight parallel Python tool to do conversion in-line with the CESM run script called pyReshaper
- Works with CESM run environment, short-term archive and XML (cesm_tseries_generator.py)
- Supports NetCDF3, NetCDF4, and NetCDF4C

# History Time-Slice to Time-Series Converter – Serial NCO

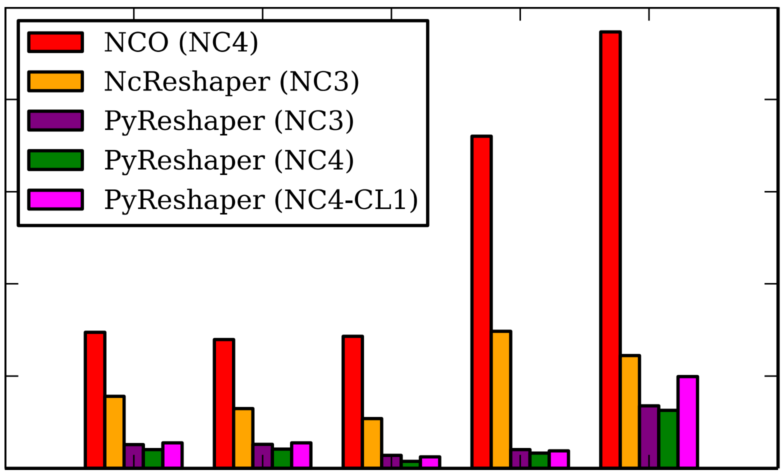


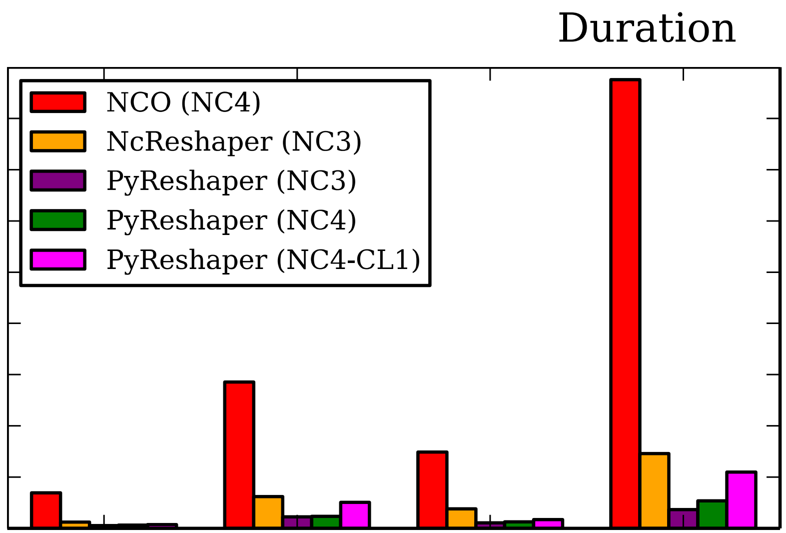
# Task Parallelization Strategy

Each rank is responsible for writing one
(or more) time-series variables to a file
pyReshaper



# Time-Series Generation Performance




Details from 1deg POP run:

- b.e12.B1850C5CN.ne30_g16.init.ch.027
- 10 years of monthly history data
- TI Metadata Variables: 63
- TV Metadata Variables: 2
- Time-Series Variables: 114
- Variables (TOTAL): 179

pyReshaper operated 4.5 times faster than NCO serial

Details from 0.1deg POP run:

- v5_rel04_BC5_ne120_t12_pop62
- 10 years of monthly history data
- TI Metadata Variables: 58
- TV Metadata Variables: 2
- Time-Series Variables: 34
- Variables (TOTAL): 94

pyReshaper operated 9 times faster than NCO serial

Yellowstone - pyReshaper used 4 nodes and 4 cores/node.

# Tasks

**Completed and available in the CESM Developer Repository:**

- New CESM Short-Term Archiving capability to local disk (st_archive) allows model to continue running concurrently with post-processing
- A Parallel Time-Series File Generator and File Compression (pyReshaper and cesm_tseries_generator.py)

**Currently Working On:**

- Bringing diagnostics and analysis capabilities into the CESM run scripts
- Automating the submission of the diagnostic packages
- Modifying diagnostic packages to be more extensible, robust, and scalable. (pyAverager)
- Archiving run metadata to the experiment database directly from the case directory for provenance. (archive_metadata)

# Diagnostic Packages

Problems:

- Runs either serially or with limited parallelization
- Not easily integrated into the CESM run environment
- Not easily extensible
- Hard to run with big data
- Only works with history time-slice data

# Solutions for the Diagnostic Packages

Reworking each package following these steps :

1. Integrate diagnostics into the CESM end-to-end automated workflow, while still maintaining stand alone capabilities
2. Diagnostic environment defined in XML
3. Creating climatology files with the PyAverager
4. Task parallelizing existing plotting scripts
5. Works with either time-slice or time-series files

# Diagnostics Integration

- Brings in the CESM case and diagnostic settings as a Python data structure
- Calls the parallel pyAverager
- Calls NCL plotting scripts in parallel
- Converts ps plots in parallel
- A directory that contains the html file and plots is created

# PyAverager Details

## A light weight custom Python averaging tool

- Parallelizes over averages and variables
- Works on time slice and time series data

## Types of averages it can compute:

- Temporal Averaging
  - Seasonal, Yearly, Annual, Monthly (weighted optional)
- Spatial Averaging
  - Across spatially split files

## Looking to also compute:

- Variance
- Across ensembles

# Time Averaging Options

- NCO (serial)
  - Controlled by a top level csh script that calls NCO operators to calculate averages.
- Swift (limited task parallel)
  - Averages are calculated in parallel calling the NCO operators
- PyAverager (task parallel)
  - New method written in Python that task parallelizes over variables and averages.

Each method was operated on both time slice and time series files

# Time Averaging Comparisons

## Datasets Used

| Component | Res | Size (GB) | # of Vars |
|---|---|---|---|
| CAM FV | 1 .0 | 28 | 139 |
| CAM SE | 1.0 | 30 | 148 |
| CAM SE | 0.25 | 1055 | 214 |
| CICE | 1.0 | 8/4 | 137 |
| CICE | 0.1 | 556/42 | 132 |
| CLM | 1.0 | 10 | 310 |
| CLM | 0.25 | 113 | 163 |
| POP | 1.0 | 190 | 170 |
| POP | 0.1 | 3113 | 87 |

* All dataset contain 10 years of both monthly time slice and time series files

## Types of time averages computed

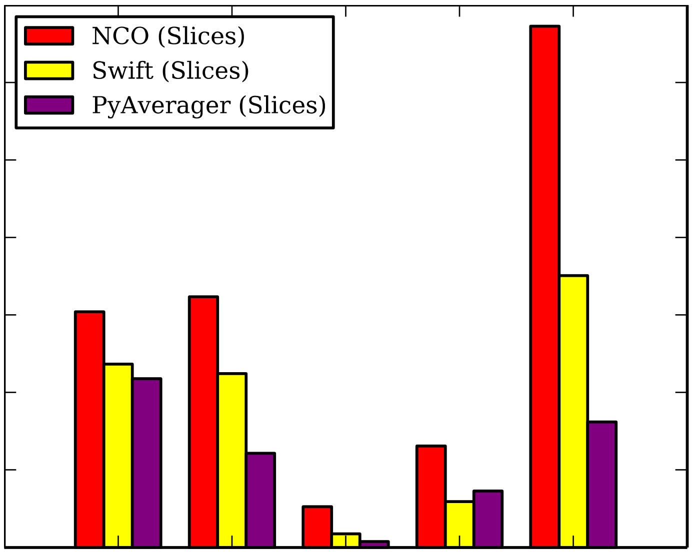
CAM & CLM

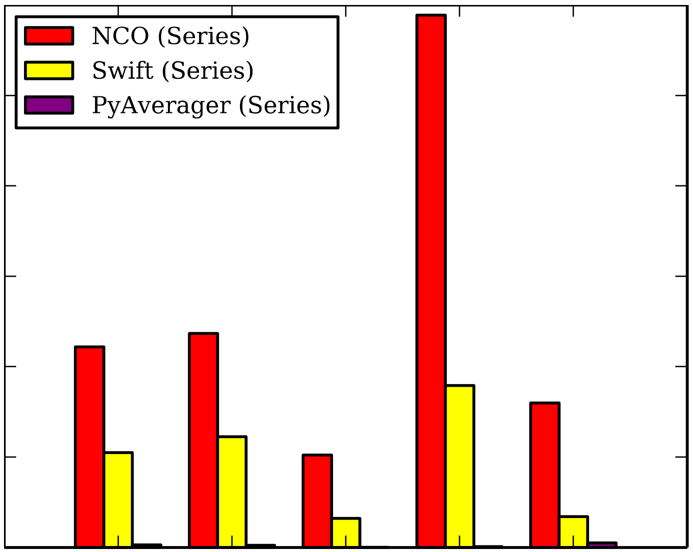
- Seasonal Averages
  - ANN,DJF,MAM,JJA,SON
- Monthly Averages
  - One average per month
- 17 Averages Total

POP & CICE

- Yearly Averages
  - One average per year
- 10 Averages Total

# Low Resolution Timings
# Original method vs. Swift vs. pyAverager

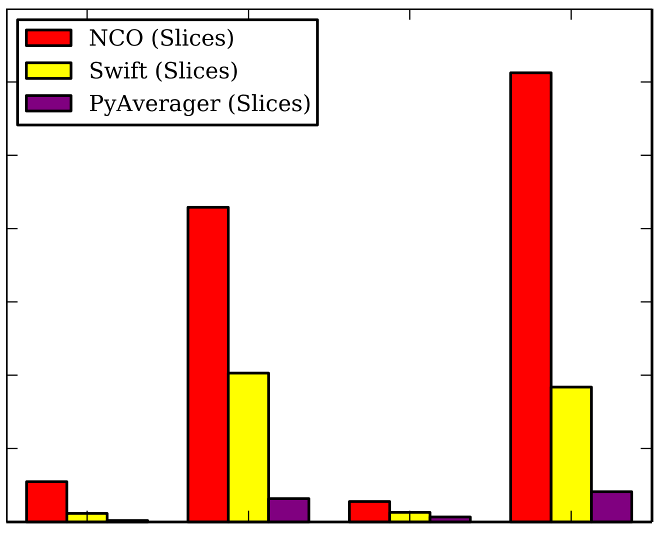


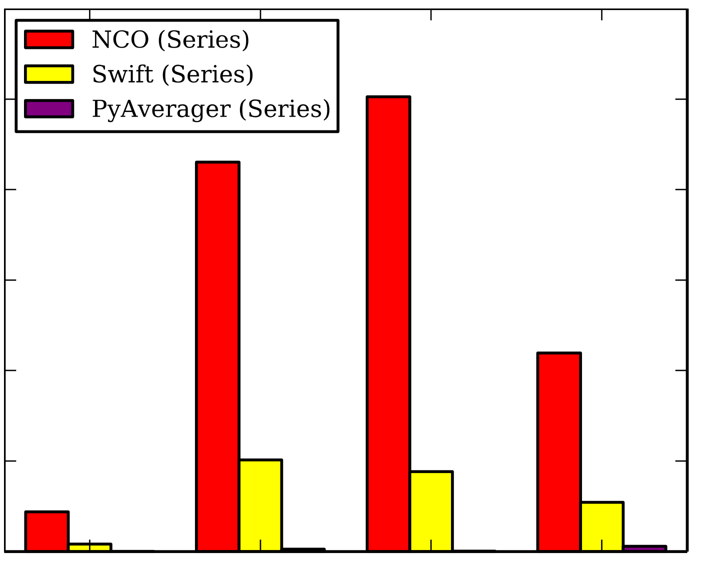




| (min) | CAM FV | CAM SE | CICE | CLM | POP |
|---|---|---|---|---|---|
| NCO | 6 | 7 | 1 | 3 | 14 |
| SWIFT | 5 | 5 | 0.4 | 1.2 | 7 |
| pyAve | 4 | 3 | 0.2 | 1.5 | 3 |

| (min) | CAM FV | CAM SE | CICE | CLM | POP |
|---|---|---|---|---|---|
| NCO | 111 | 118 | 51 | 295 | 80 |
| SWIFT | 53 | 61 | 16 | 90 | 17 |
| pyAve | 2 | 1 | 0.1 | 0.4 | 3 |

# High Resolution Timings
# Original method vs. Swift vs. pyAverager




| (min) | CICE | CAM | CLM | POP |
|---|---|---|---|---|
| NCO | 27 | 215 | 14 | 306 |
| SWIFT | 6 | 102 | 7 | 92 |
| pyAve | 1 | 16 | 4 | 21 |

| (min) | CICE | CAM | CLM | POP |
|---|---|---|---|---|
| NCO | 88 | 861 | 1005 | 439 |
| SWIFT | 16 | 203 | 177 | 109 |
| pyAve | 0.2 | 5 | 0.7 | 12 |

# Computational Resources Used For Timing Comparisons

| File Type | NCO-Slice | NCO-Series | Swift-Slice | Swift-Series | PyAvg-Slice | PyAvg-Series |
|---|---|---|---|---|---|---|
| POP-1.0 | Y/1 | Y/1 | G/16 | G/16 | Y/160 | Y/160 |
| CLM-1.0 | Y/1 | Y/1 | G/16 | G/16 | Y/160 | Y/160 |
| CICE-1.0 | Y/1 | Y/1 | G/16 | G/16 | Y/160 | Y/160 |
| CAMSE-1.0 | Y/1 | Y/1 | G/16 | G/16 | Y/160 | Y/160 |
| CAMFV-1.0 | Y/1 | Y/1 | G/16 | G/16 | Y/160 | Y/160 |
| POP-0.1 | BM/1 | Y/1 | BM/4 | G/16 | G/40 | G/40 |
| CLM-0.25 | GP/1 | Y/1 | G/16 | G/16 | Y/160 | Y/160 |
| CICE-0.1 | GP/1 | Y/1 | G/16 | G/16 | Y/160 | Y160 |
| CAM-0.25 | GP/1 | Y/1 | G/16 | G/16 | Y/160 | Y/160 |

Machine/Cores
Y=Yellowstone  G=Geyser  GP=GPGPU  BM=BigMem

# CSEG Support

- CESM Users Guide updates
- XML modifications via existing tools
- DiscussCESM bulletin board forums
- Coordination with LIMWG and PCWG
  - Diagnostics packages
- Coordination with CISL
  - Parallel Python tools

# Continued Work

- Extending the flexibility of the run scripts
- Creating more extensible working environments
- Providing solutions to increase scalability and automation within the workflow
  - Including other CMIP workflow tools
- Adding testing into the current post-process workflow

# Questions?

**CESM workflow refactor team**

- Ben Andre
- Alice Bertini
- John Dennis
- Jim Edwards
- Mary Haley
- Jean-Francois Lamarque
- Michael Levy
- Sheri Mickelson
- Kevin Paul
- Sean Santos
- Jay Shollenberger
- Gary Strand
- Mariana Vertenstein