CESM Workflow Refactor Project
OMWG 2015 Winter Meeting

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CSEG & ASAP/CISL

CESM Workflow Refactor Project

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

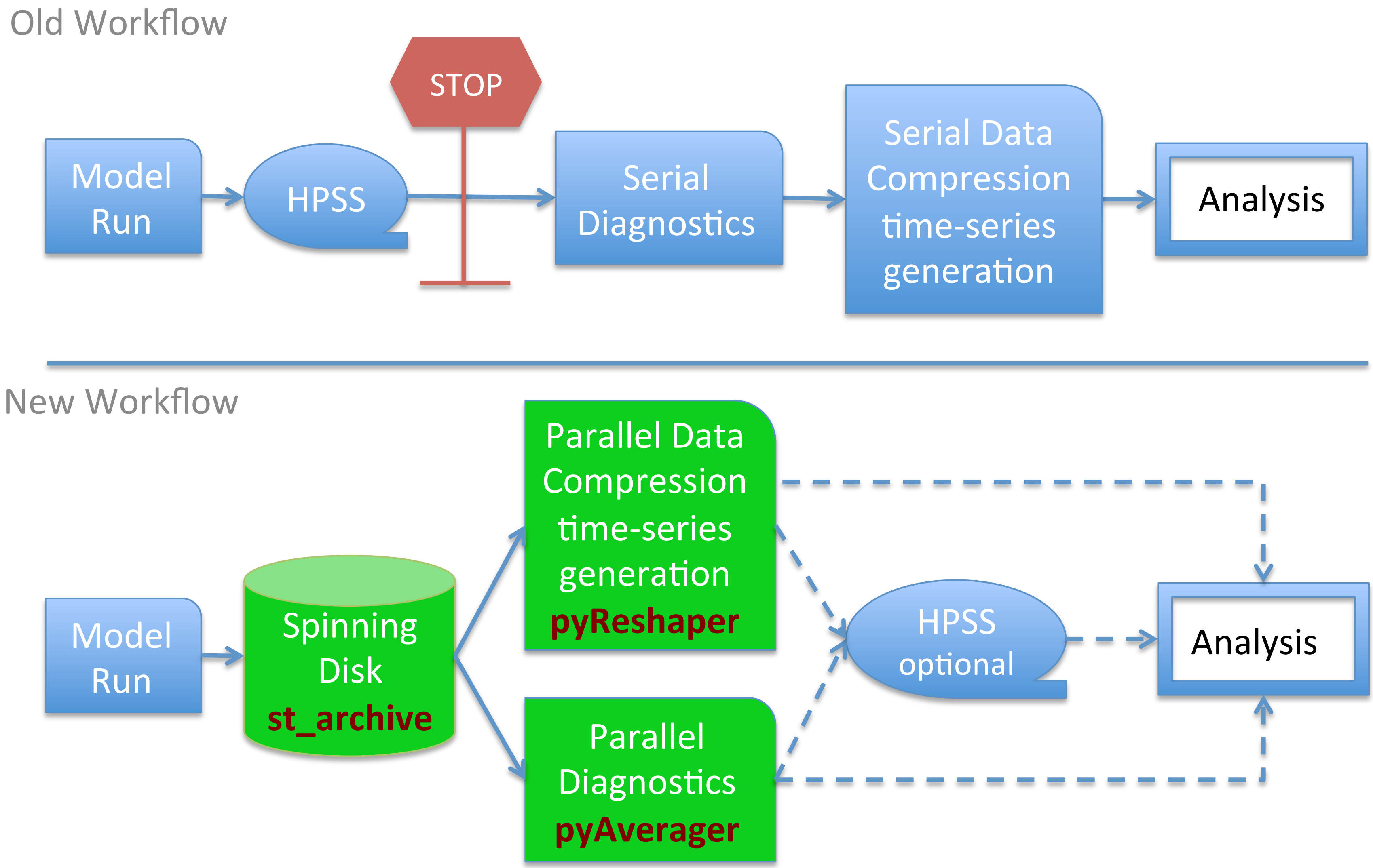
Goals? To create a new end to end workflow that enables scientists to get work done easier and faster

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

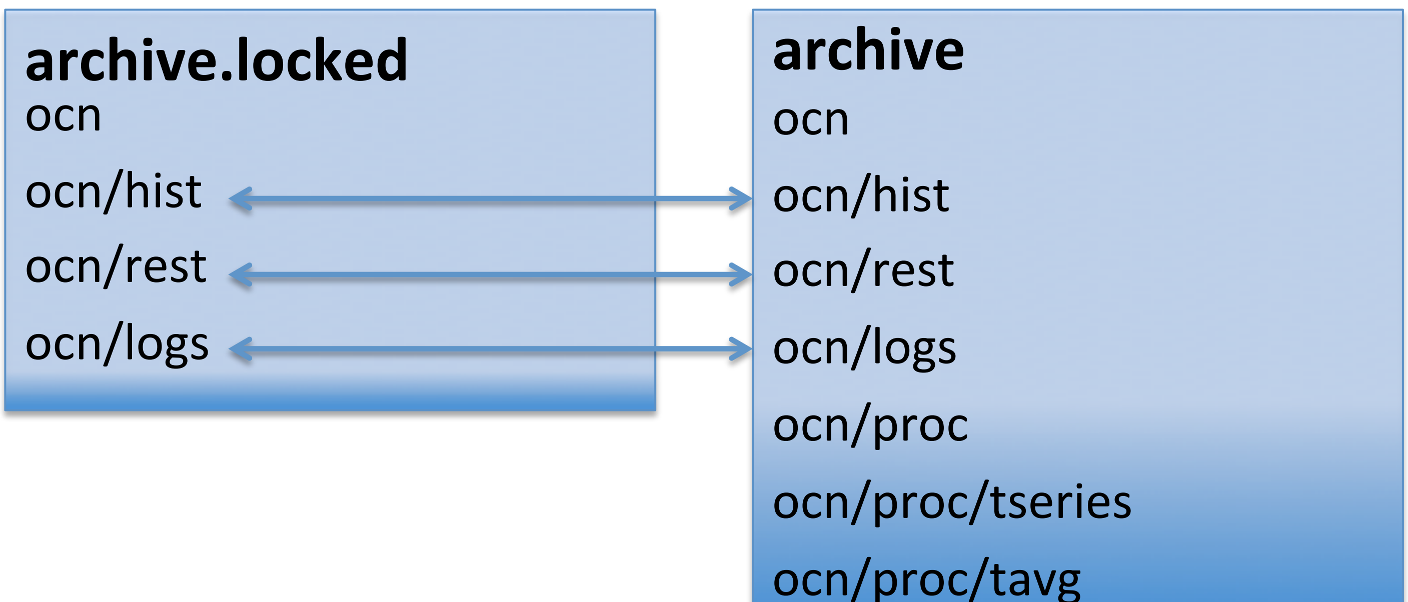
Solution:

- 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

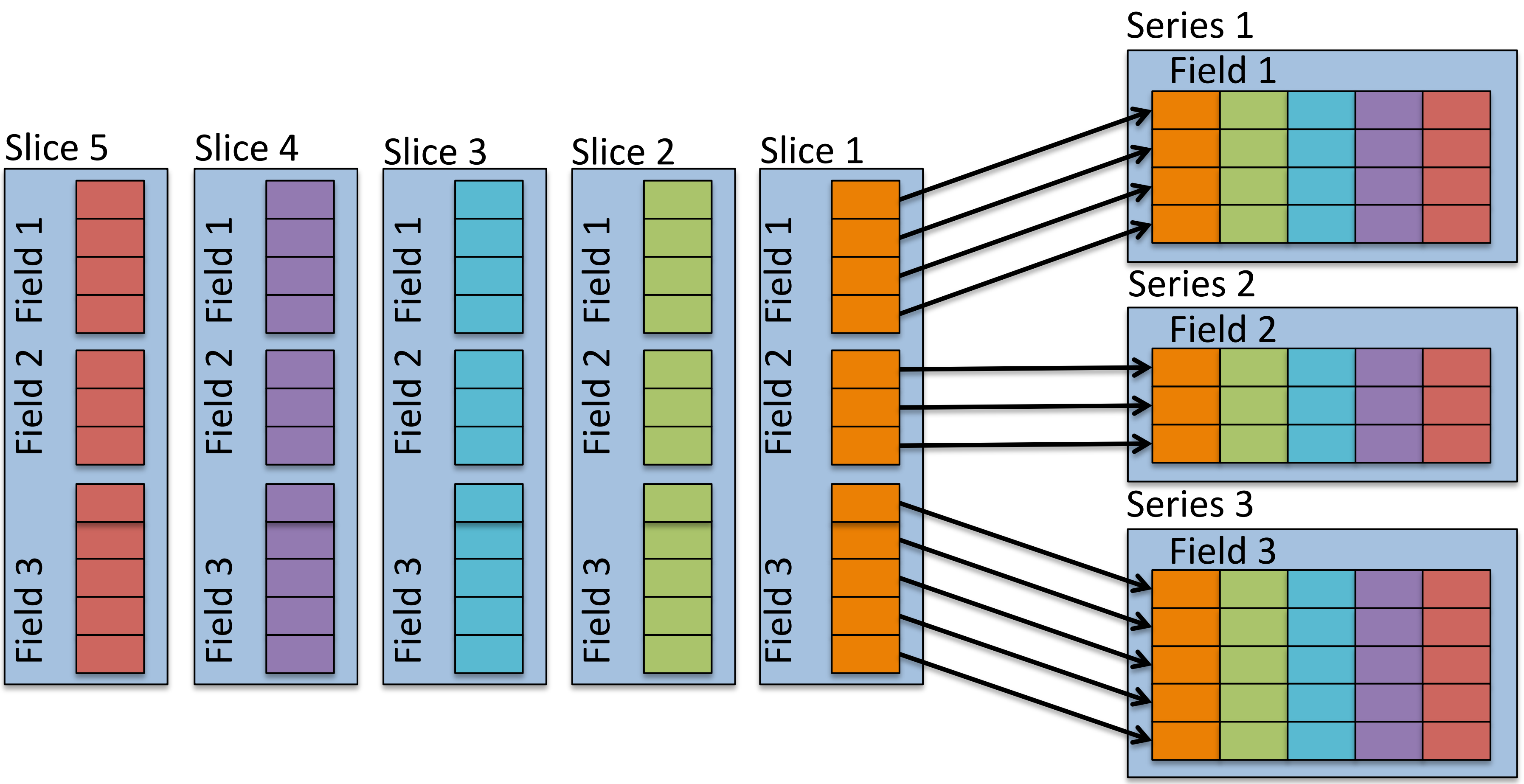
Problems:

- 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:

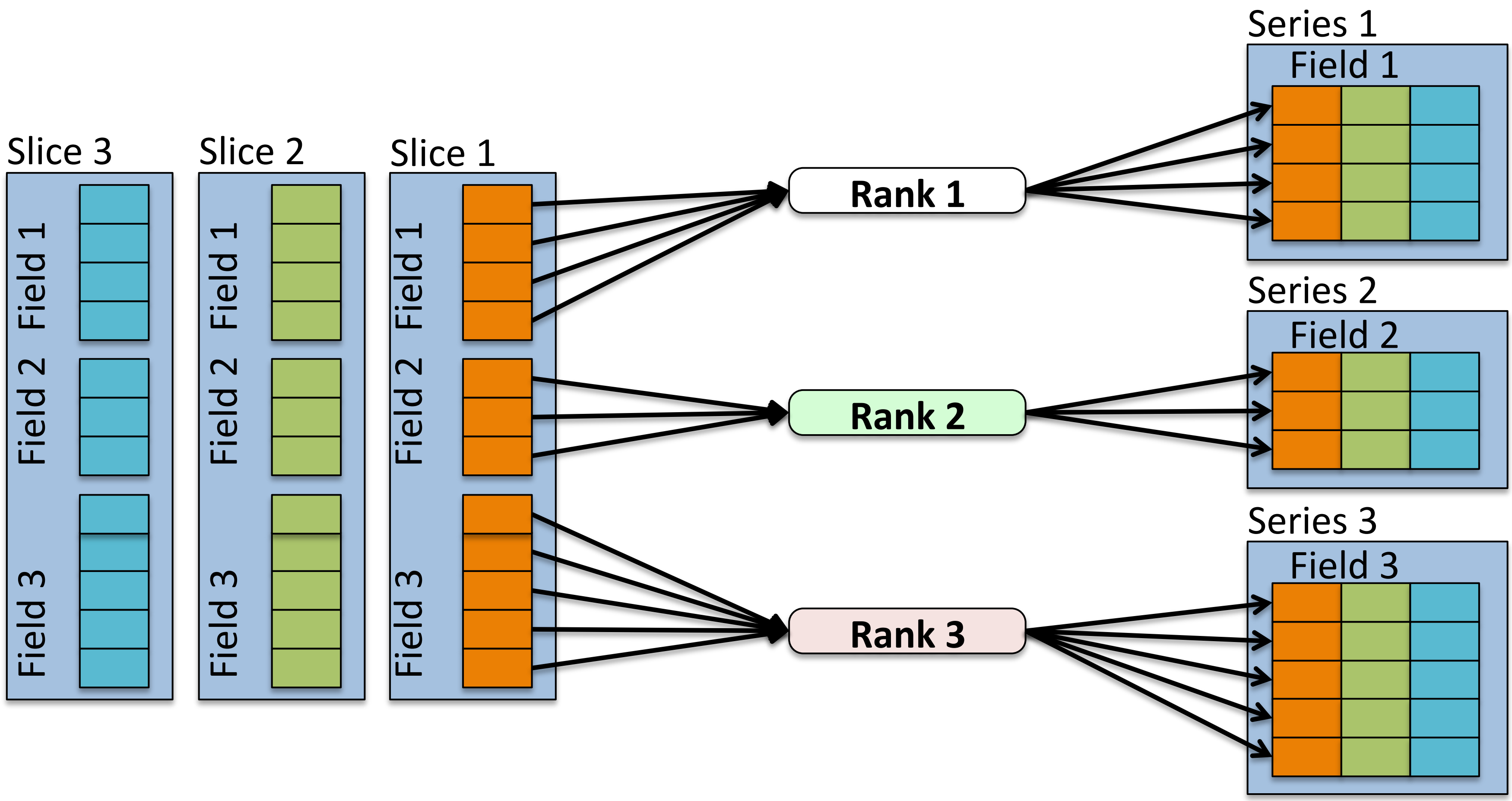
- Light-weight parallel Python tool to do conversion in-line with the CESM run script called pyReshaper
- Works with CESM run environment, short-term archive and XML (cesm_tseries_generator.py)
- Supports NetCDF3, NetCDF4, and NetCDF4C

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

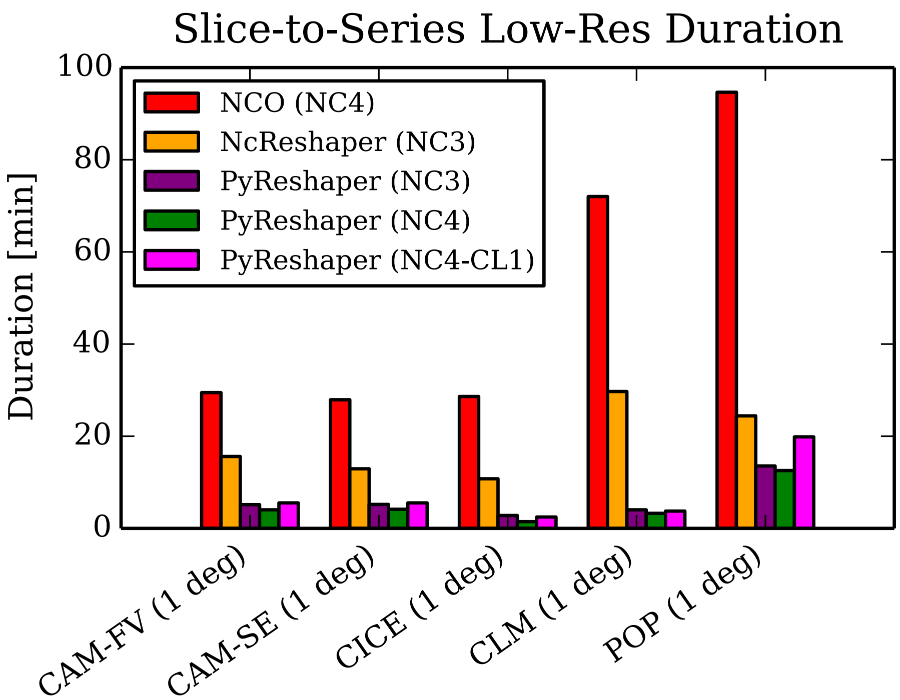


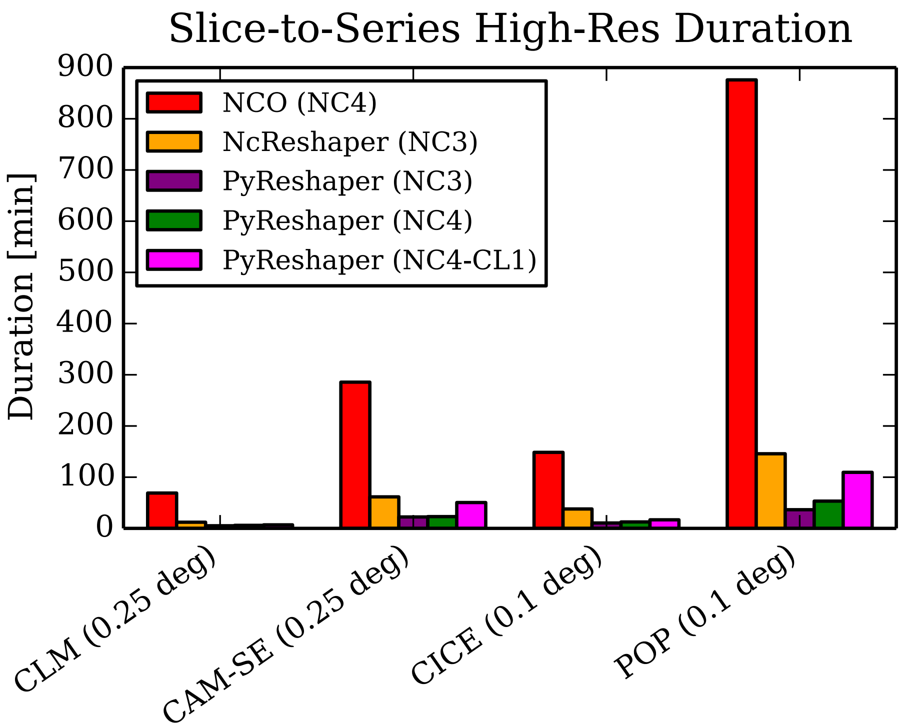
Task Parallelization Strategy

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 workflow
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

Focusing on the AMWG, OMWG, Land, and Ice Diagnostic Packages

OMWG Diagnostics Integration

Python wrapper script ocn_diags_generator.py

(Replaces popdiag.csh, popdiagdiff.csh, popdiagts.csh)

- Brings in the CESM case and diagnostic settings as a Python data structure
- Calls the parallel pyAverager
- Calls NCL plotting scripts in parallel
- Converts plots from ps to gif 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

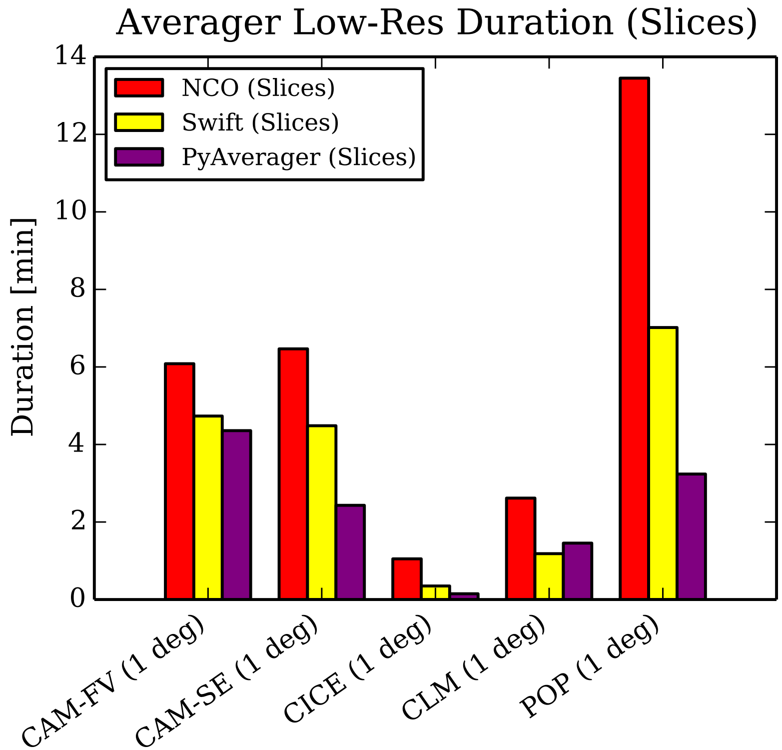
CAM & CLM

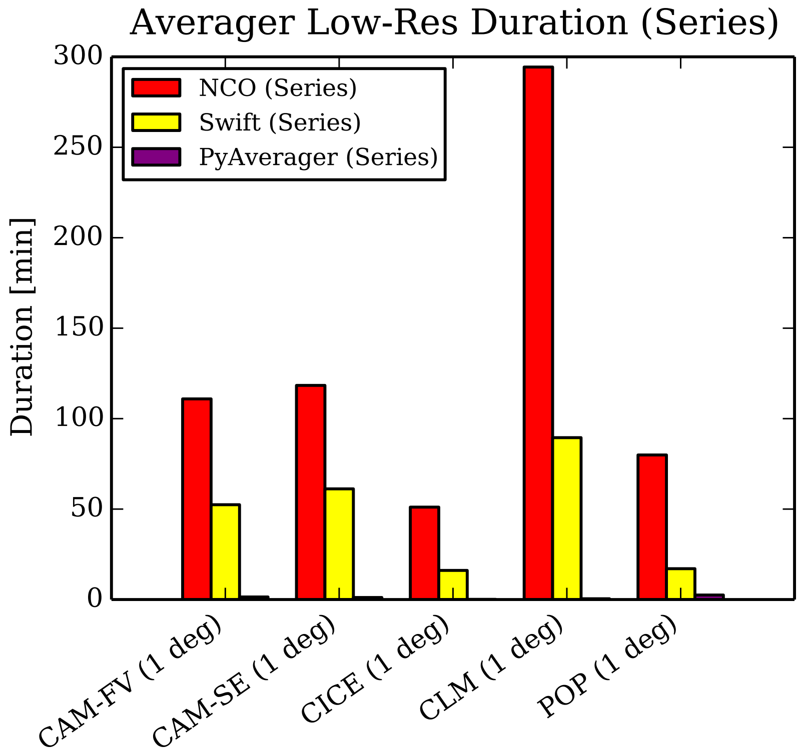
- Seasonal Averages
  - ANN,DJF,MAM,JJA,SON
- Monthly Averages
  - One average per month
- 17 Averages Total

POP & CICE

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

Low Resolution Timings
Original method vs. Swift vs. pyAverager

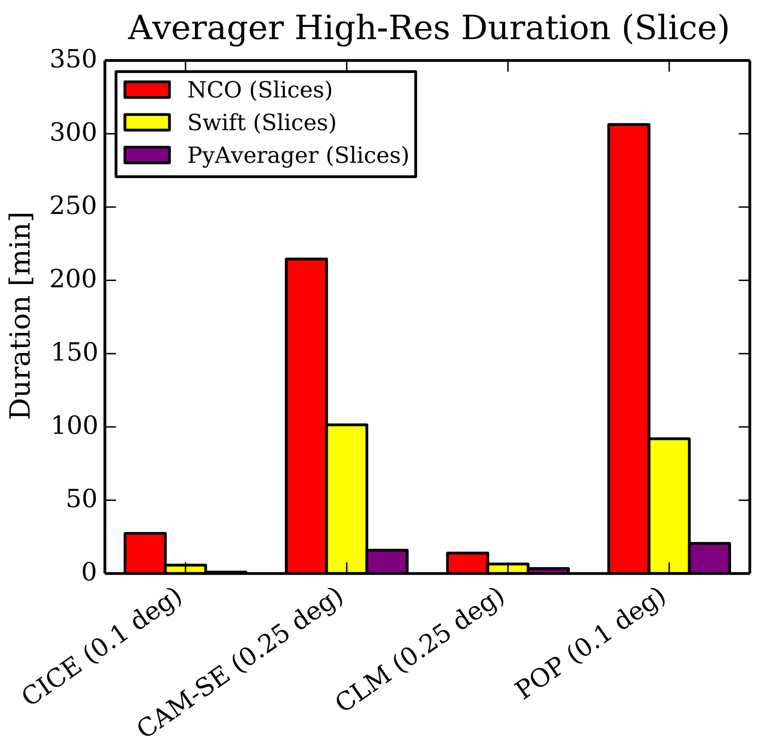


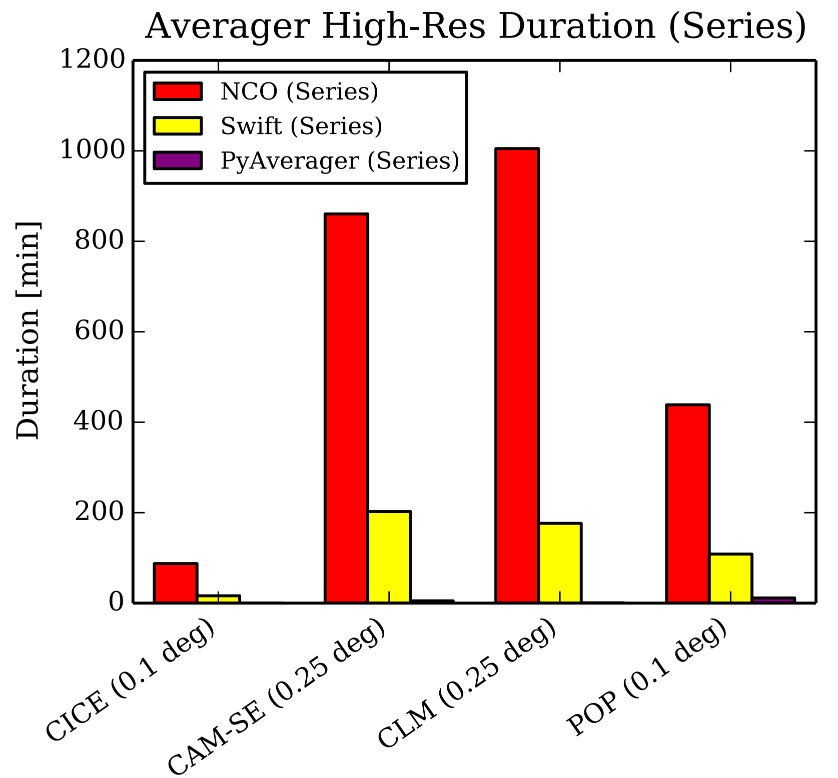


(min)	CAM FV	CAM SE	CICE	CLM	POP
NCO	6	7	1	3	14
SWIFT	5	5	0.4	1.2	7
pyAve	4	3	0.2	1.5	3

(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 OMWG
  - Popdiag specific tools (i.e. za – zonal average)
  - NCL, IDL, and Python plotting scripts
  - Additional OMWG specific features
- Coordination with CISL
  - Parallel Python tools

Continued Work

- Extending the flexibility of the run scripts
- Providing modular and extensible working environments
- Providing solutions to increase scalability within the workflow
- Adding testing into the current workflow

Continue the effort to make running the end to end CESM workflow easier and faster so more science can be done

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