Light-Weight Parallel Python Tools for Earth System Modeling Workflows

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NCAR

NSF

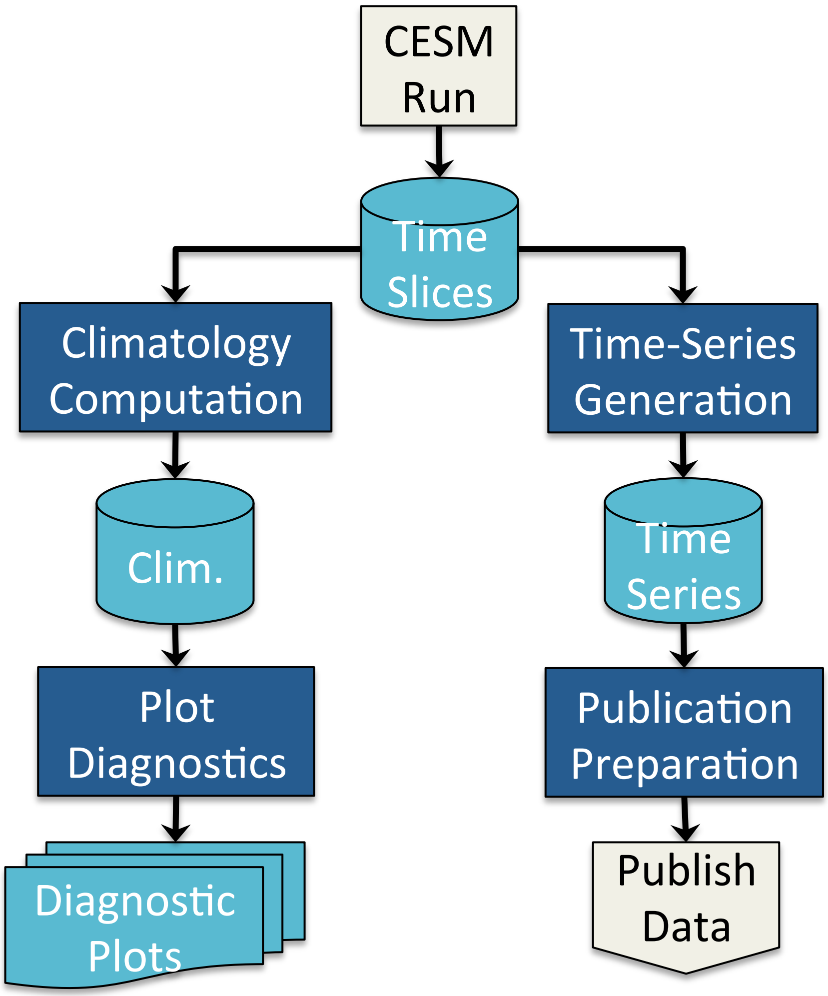
The Problem

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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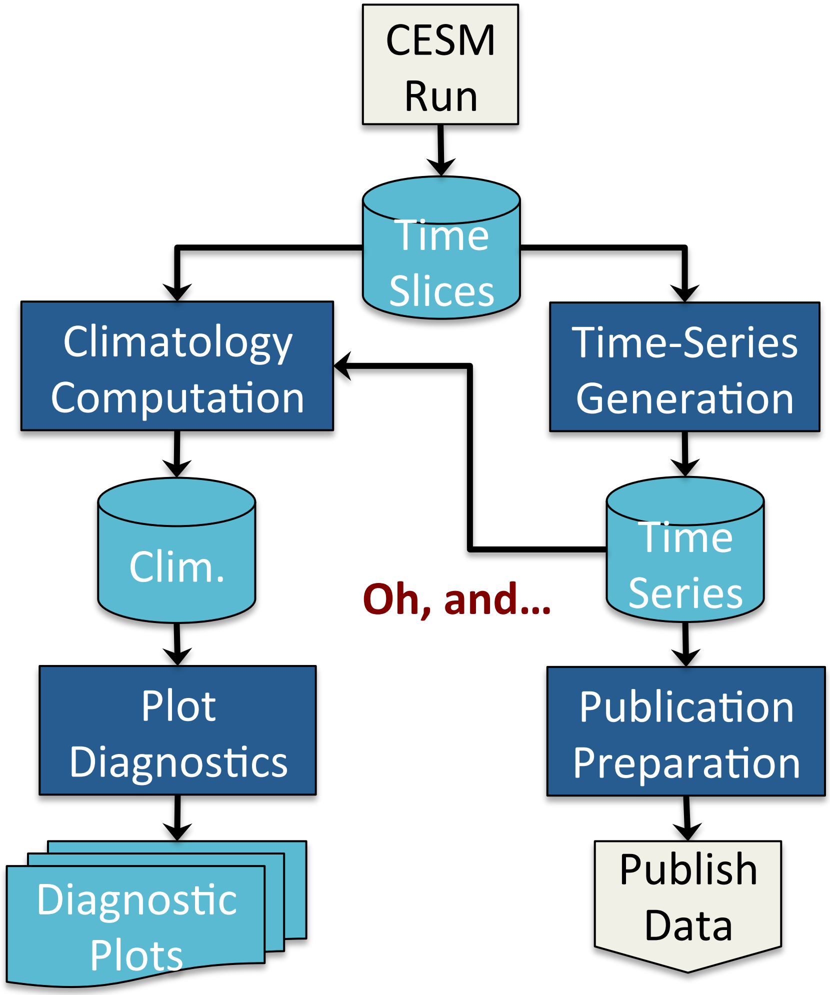

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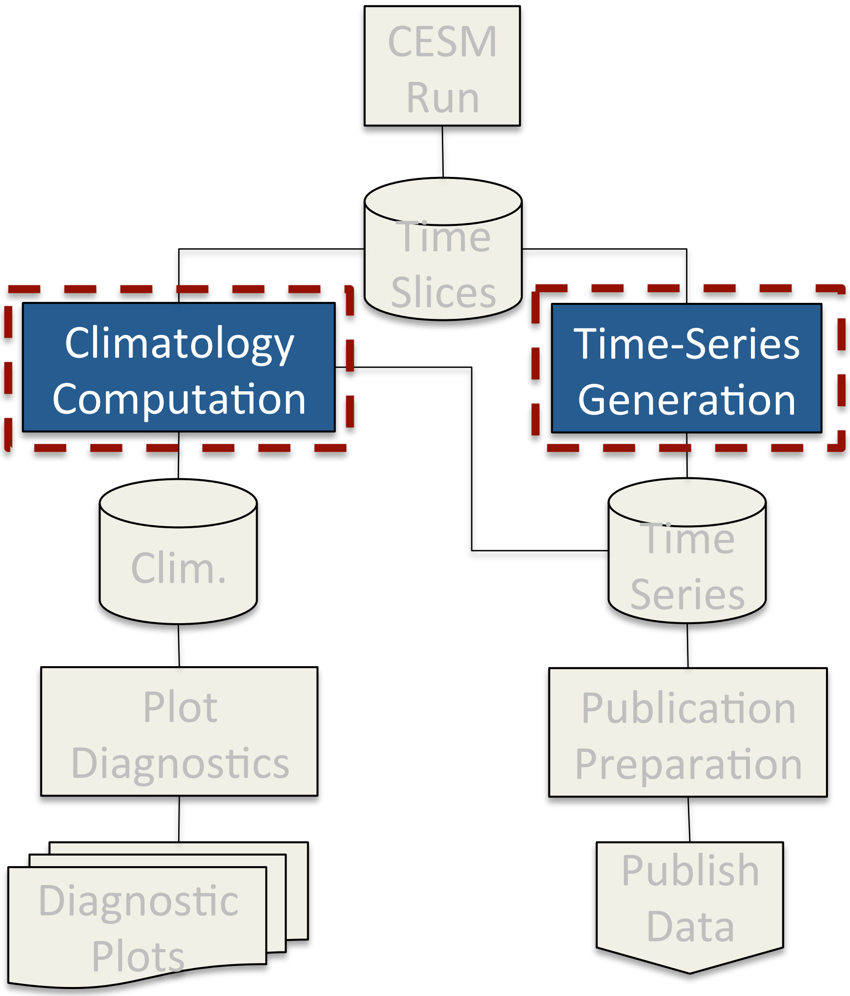


Approach & Design

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

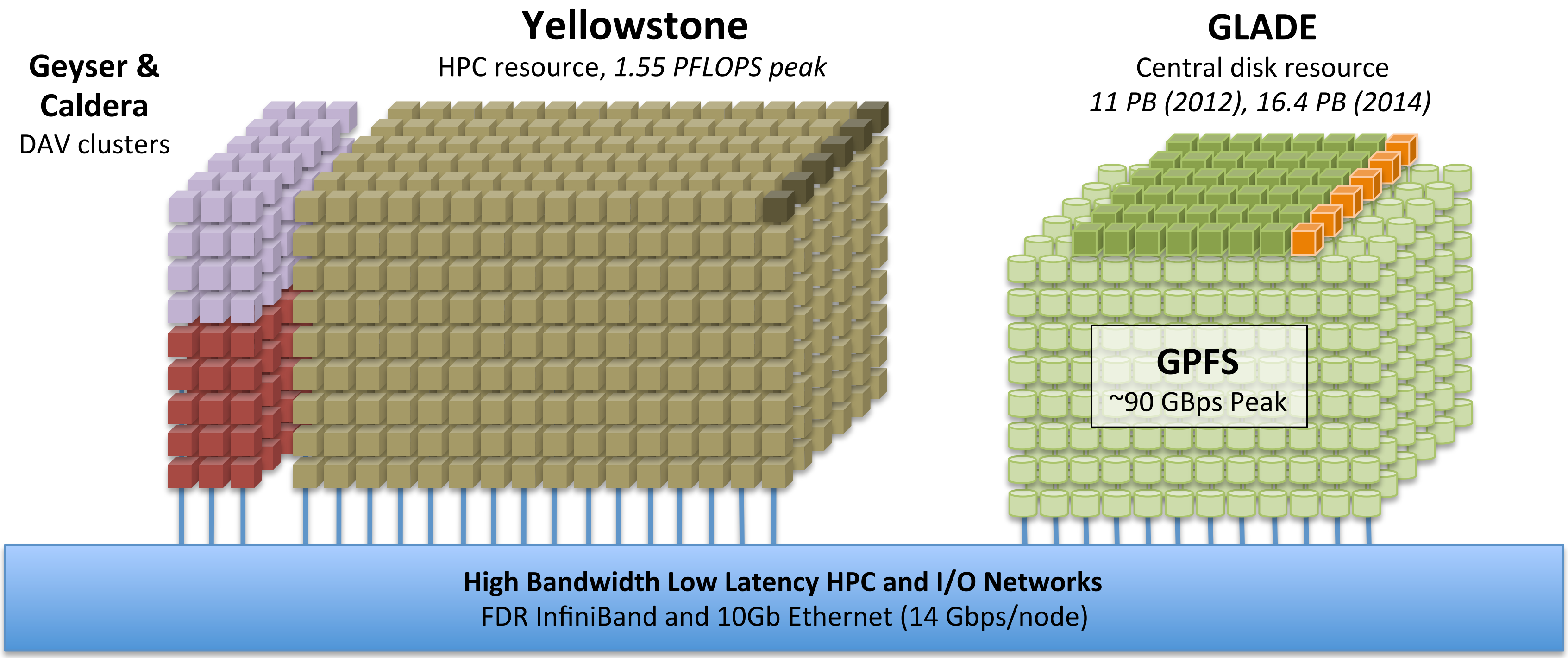
Testing

Testing Datasets

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

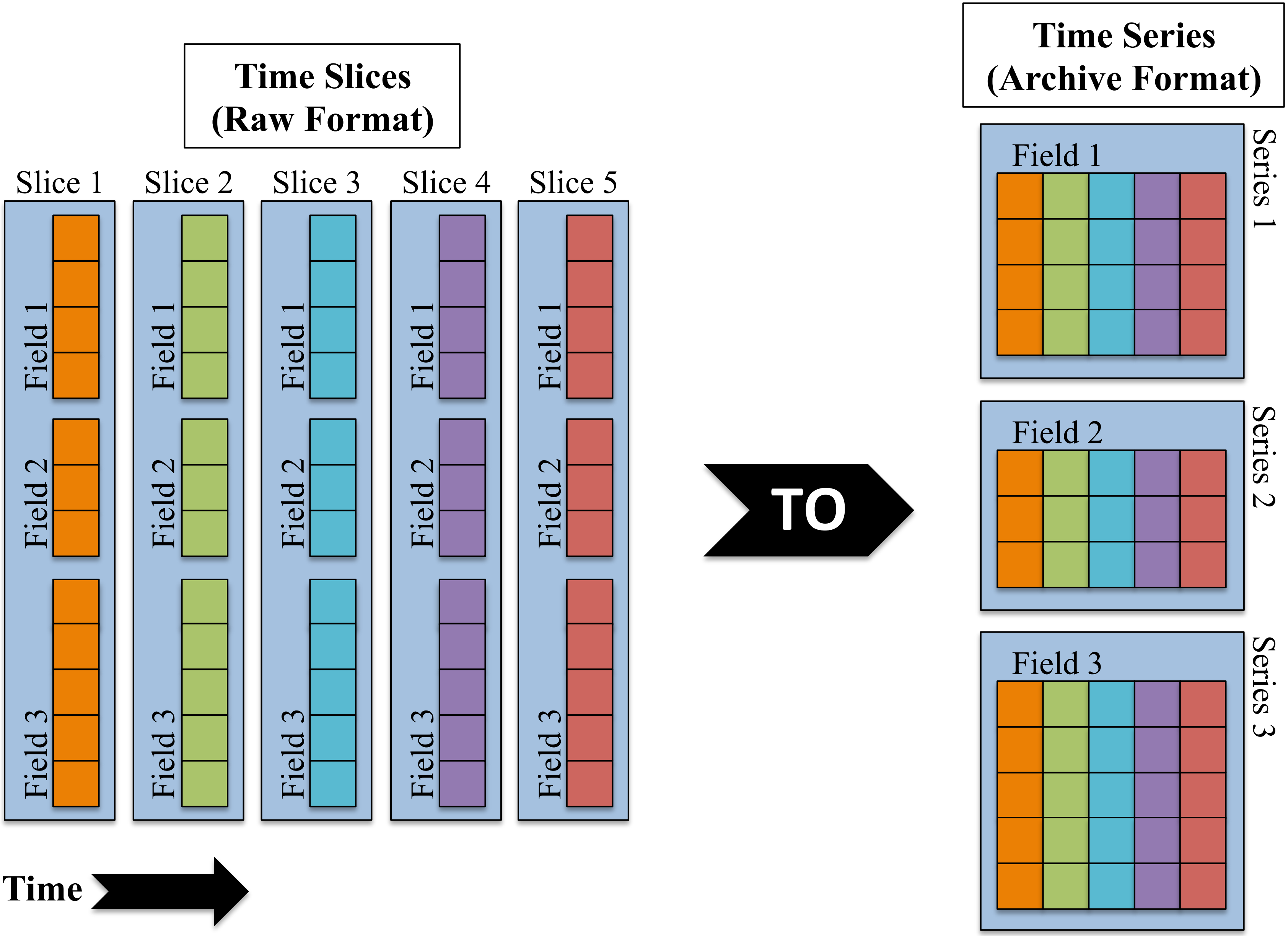
- Datasets span 10 years of monthly data

Testing Platform

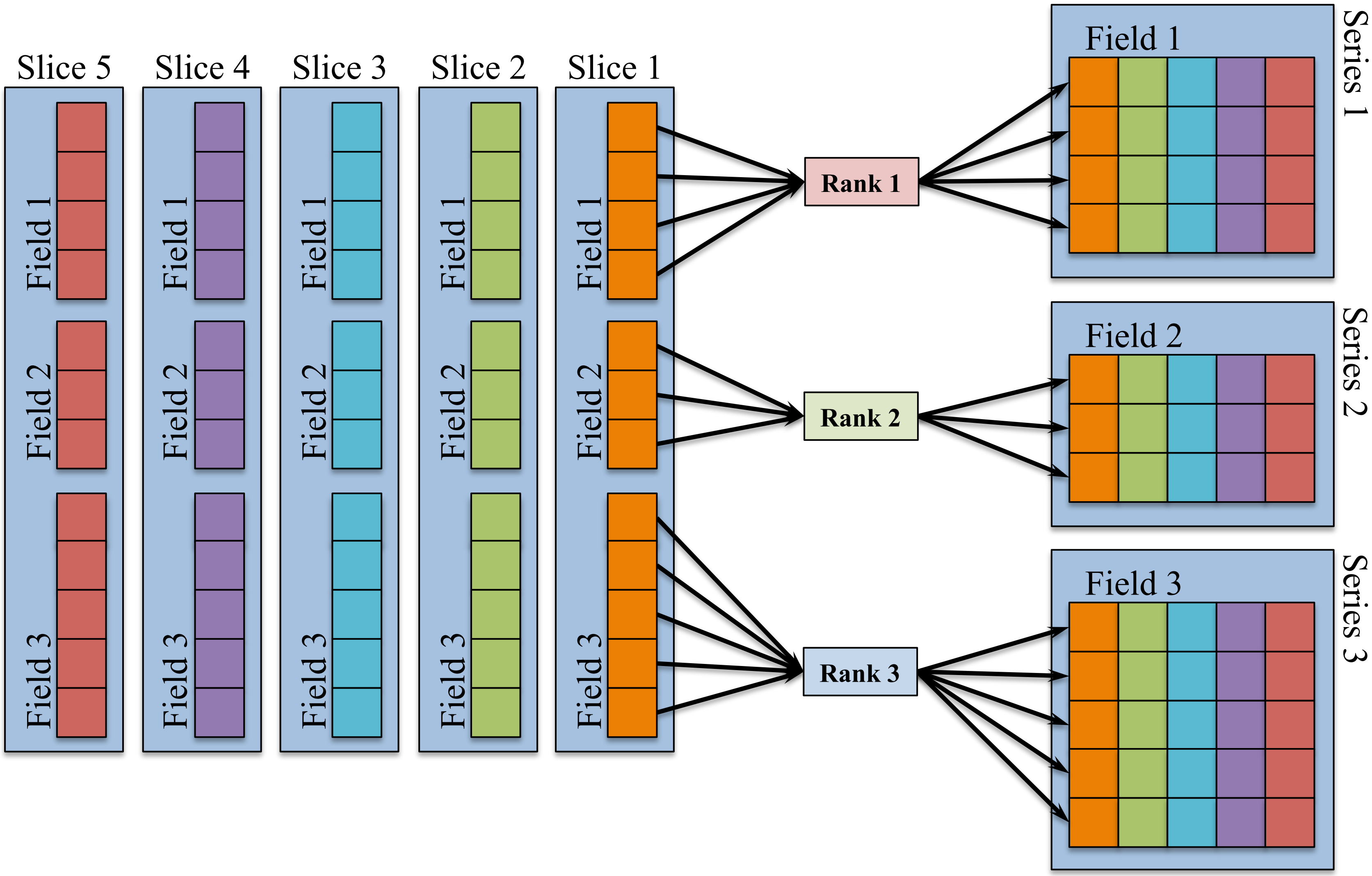


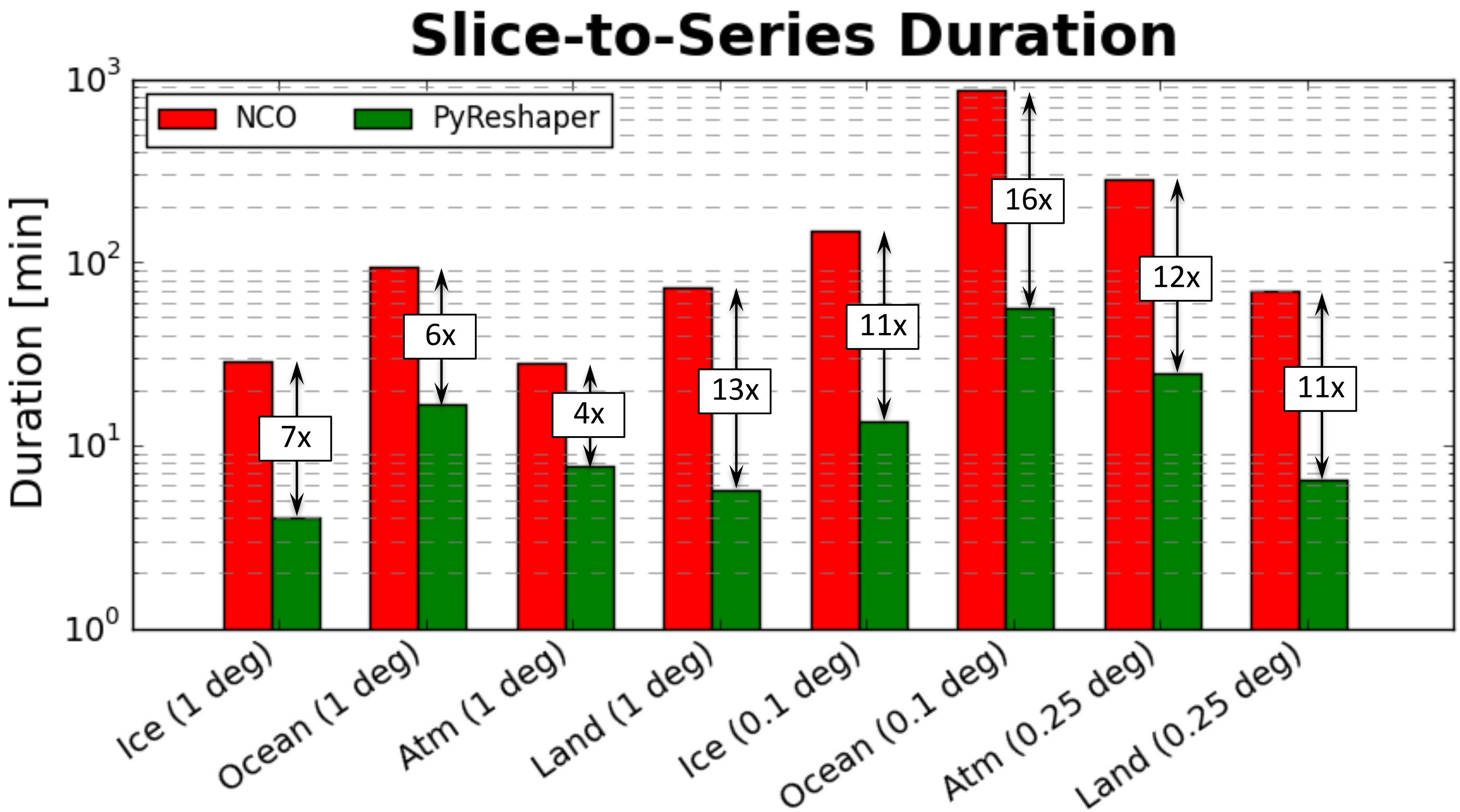
- NCAR's Yellowstone, GLADE & GPFS:
  - ~90 GB/s peak from GPFS
  - ~1.5 GB/s from each compute node

The PyReshaper: "Time-Series Generation"

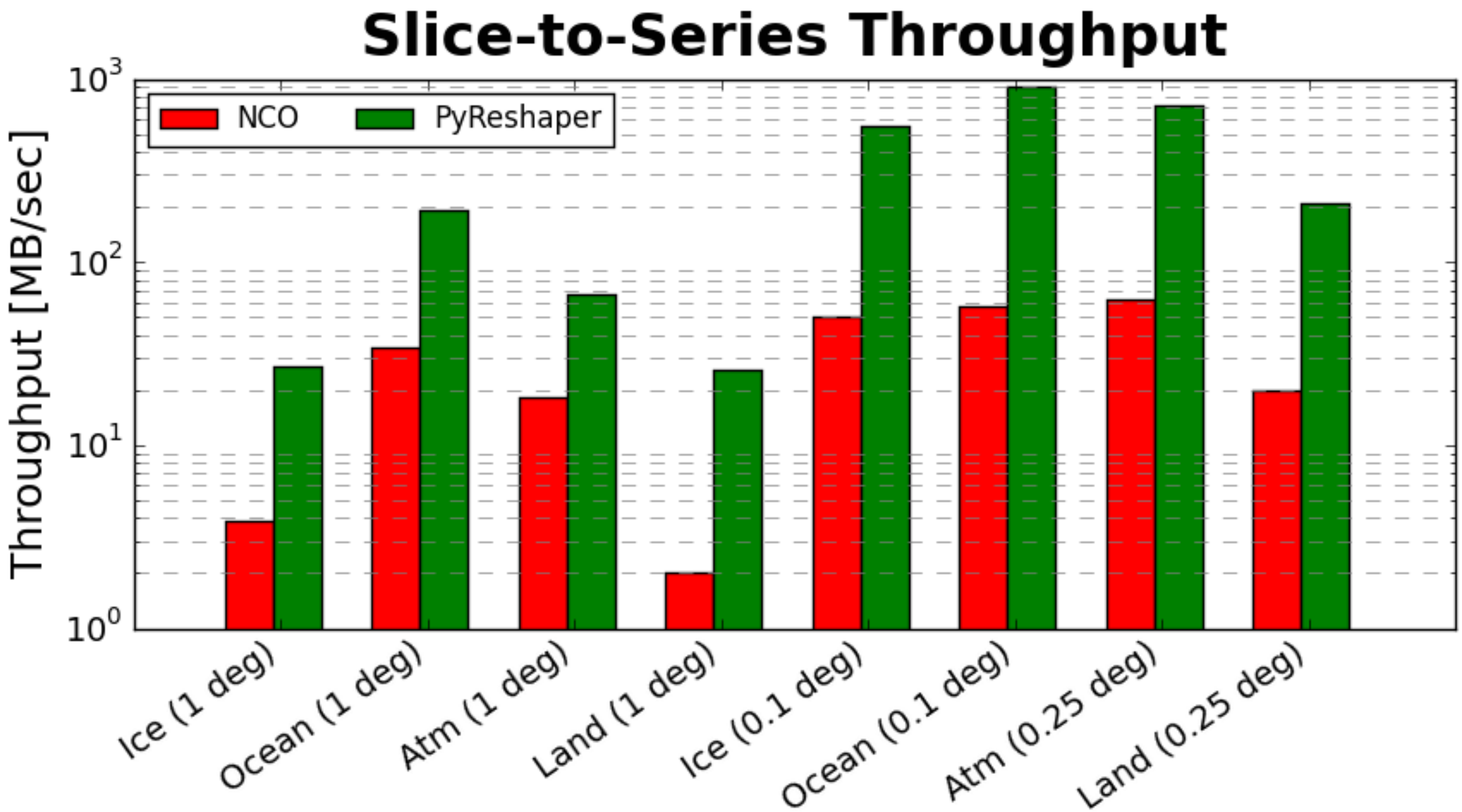

Time Slices
(Raw Format)
Slice 1
Slice 2
Slice 3
Slice 4
Slice 5
Field 1
Field 2
Field 3
Time
TO
Time Series
(Archive Format)
Field 1
Series 1
Field 2
Series 2
Field 3
Series 3

Task Parallelism





- 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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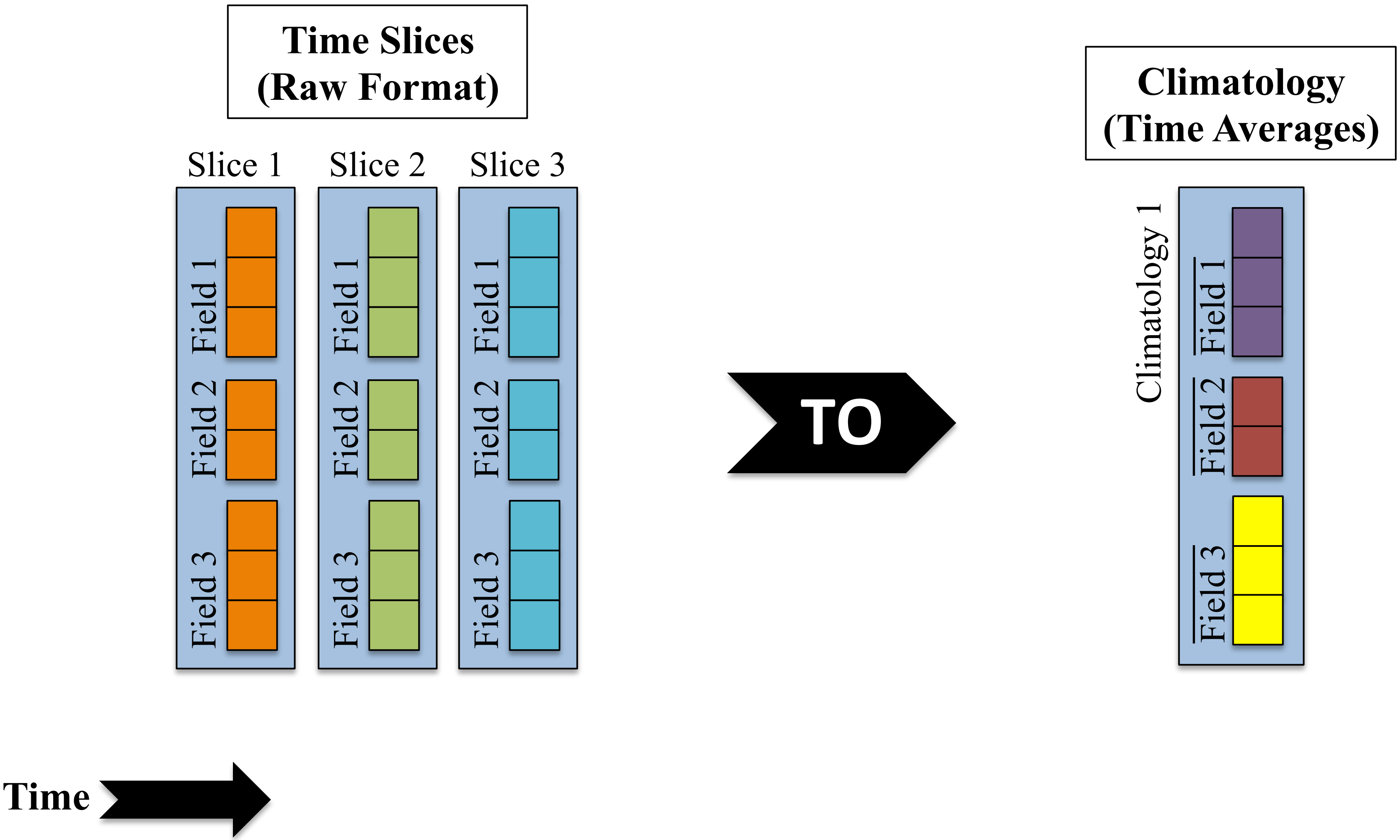
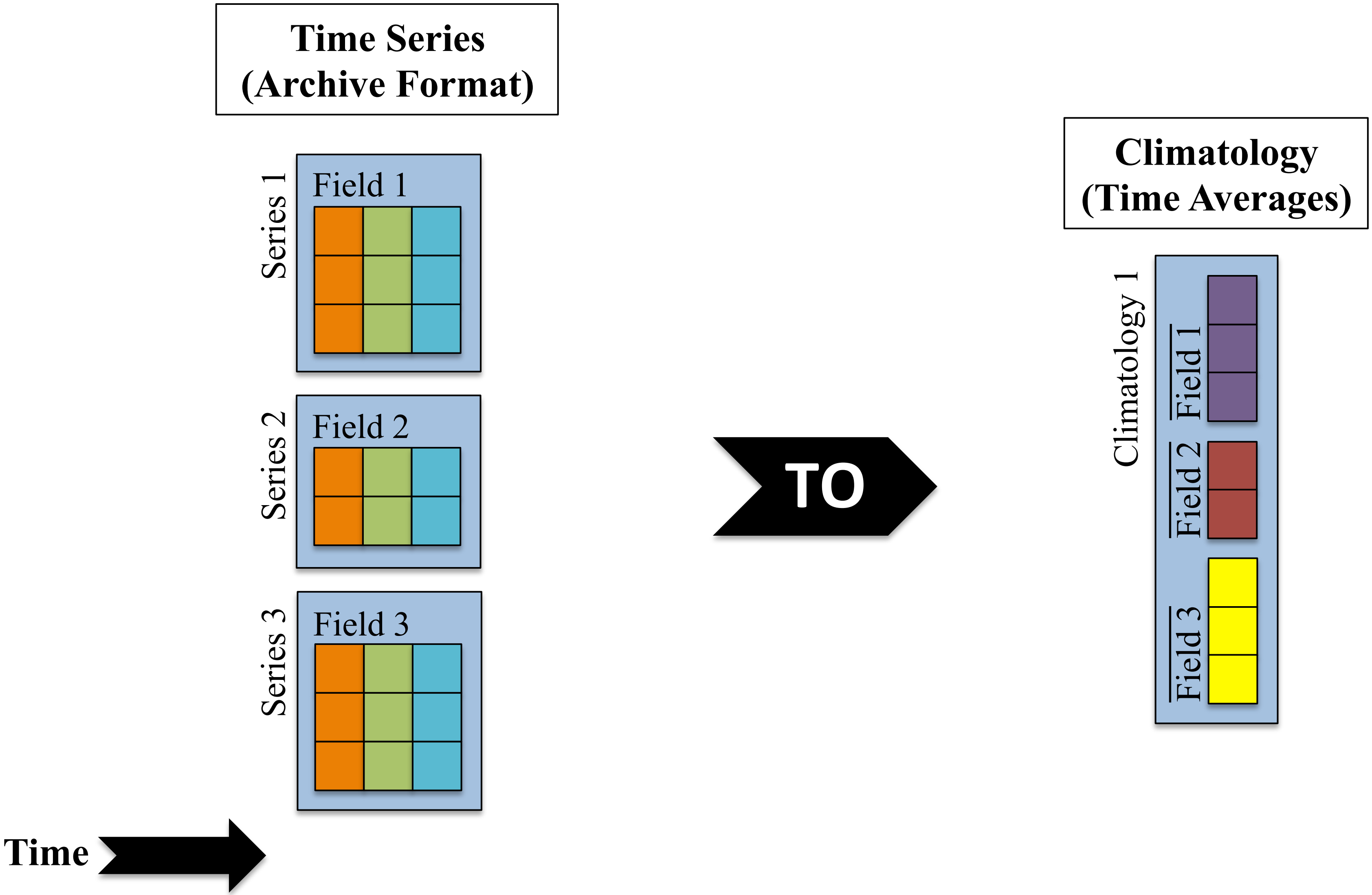
The PyAverager:
“Climatology Computation”


Time Slices
(Raw Format)
Slice 1
Slice 2
Slice 3
Field 1
Field 2
Field 3
TO
Climatology
(Time Averages)
Climatology 1
Field 1
Field 2
Field 3
Time


Time Series
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Series 1
Field 1
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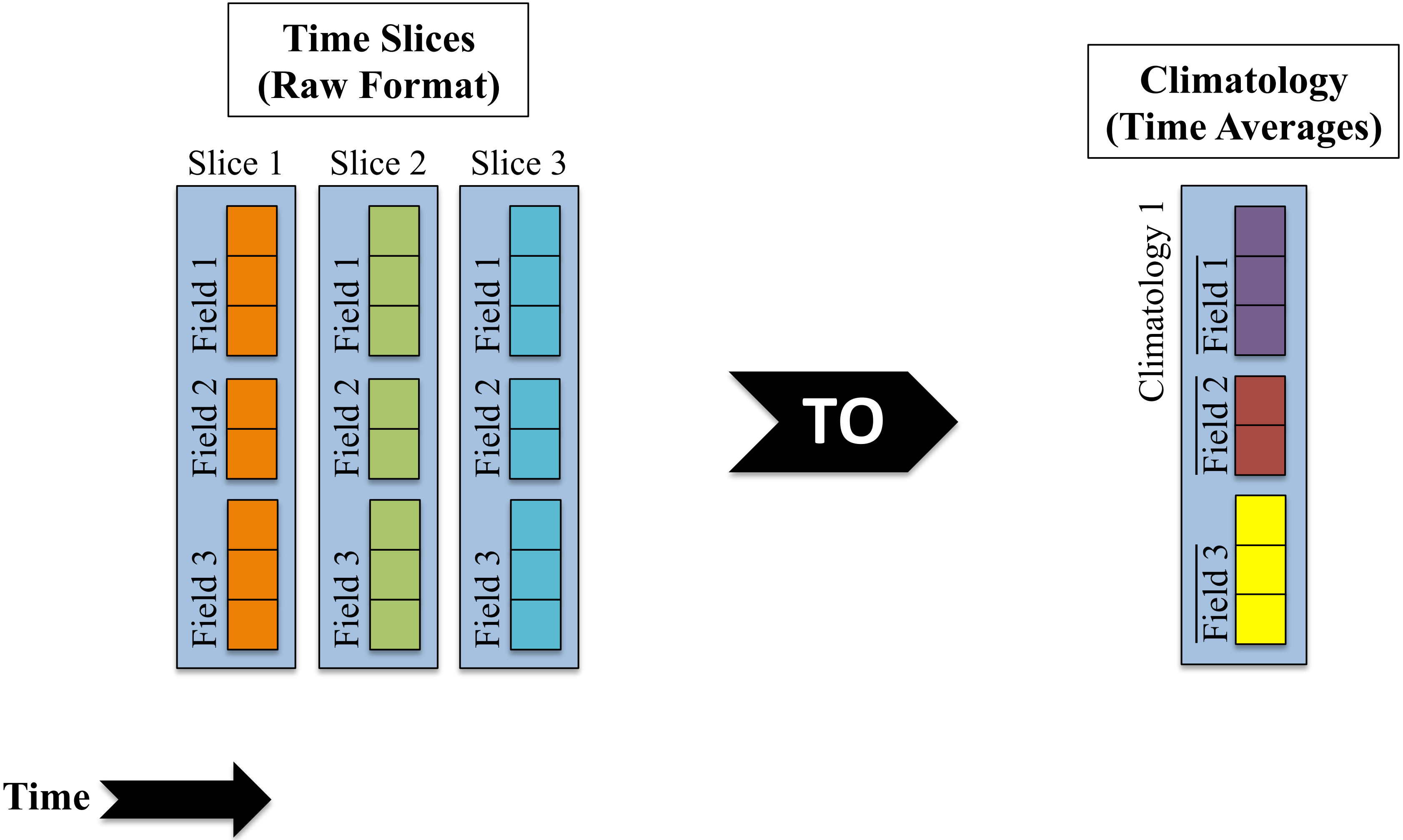
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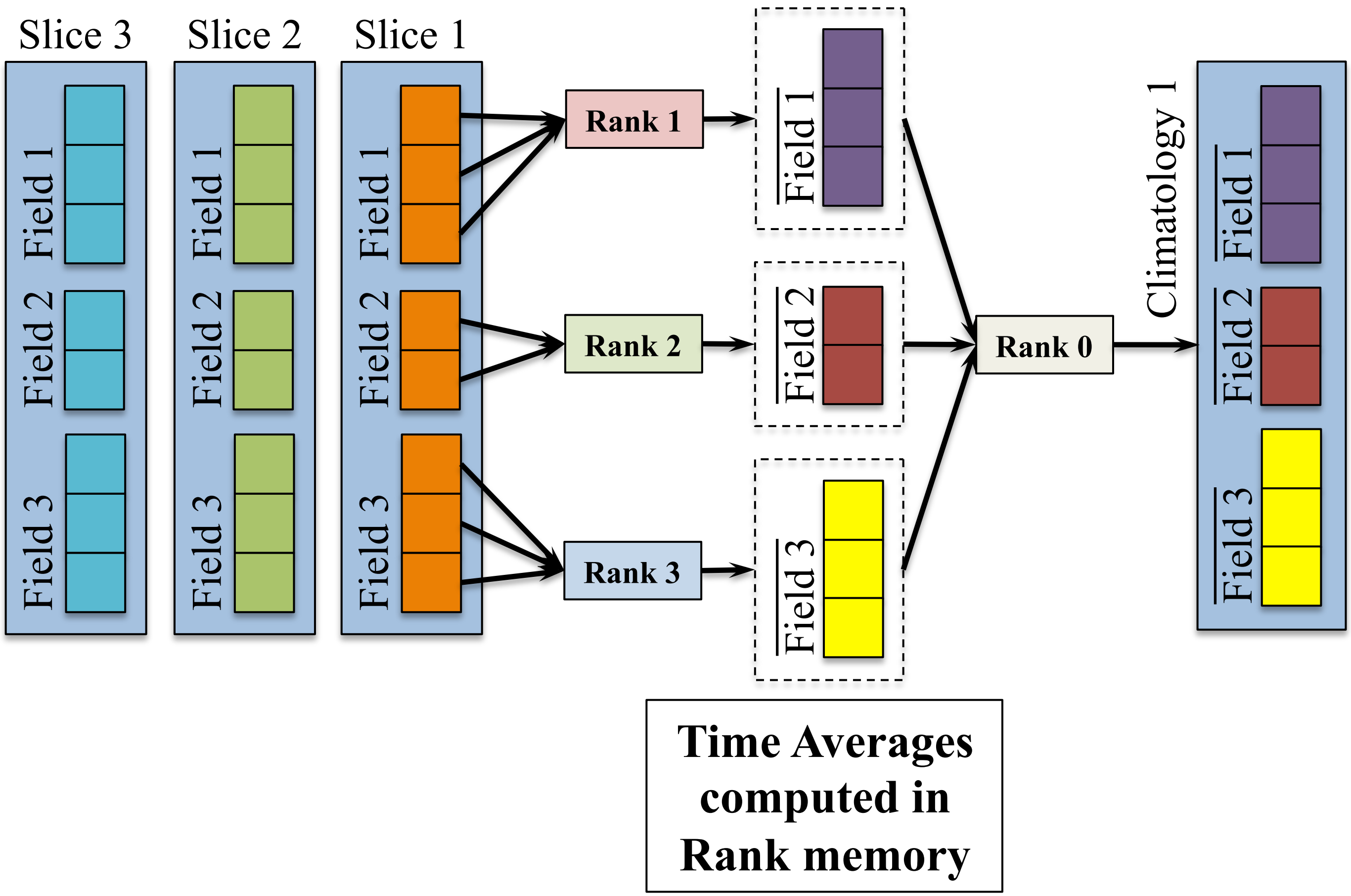
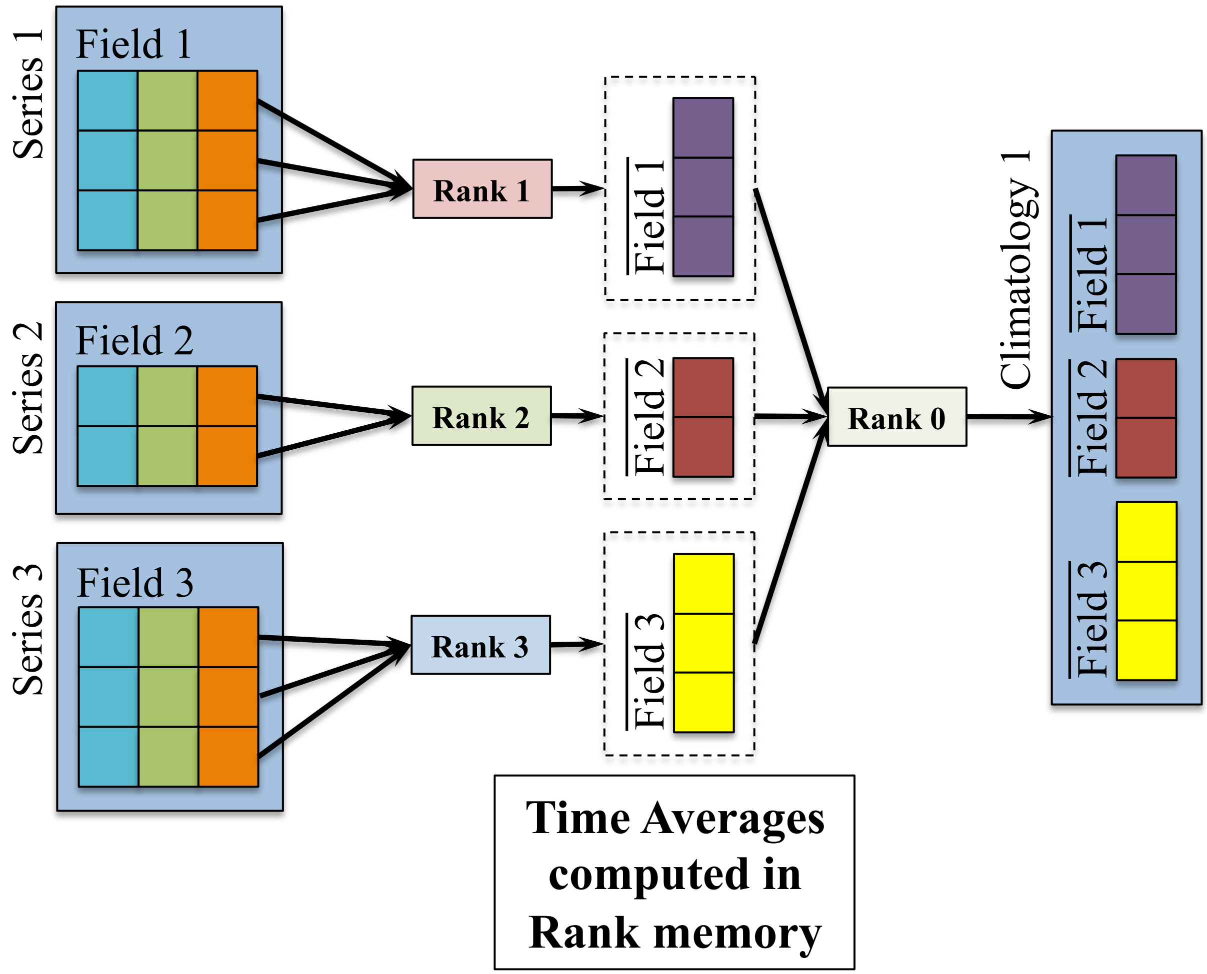
Task Parallelism

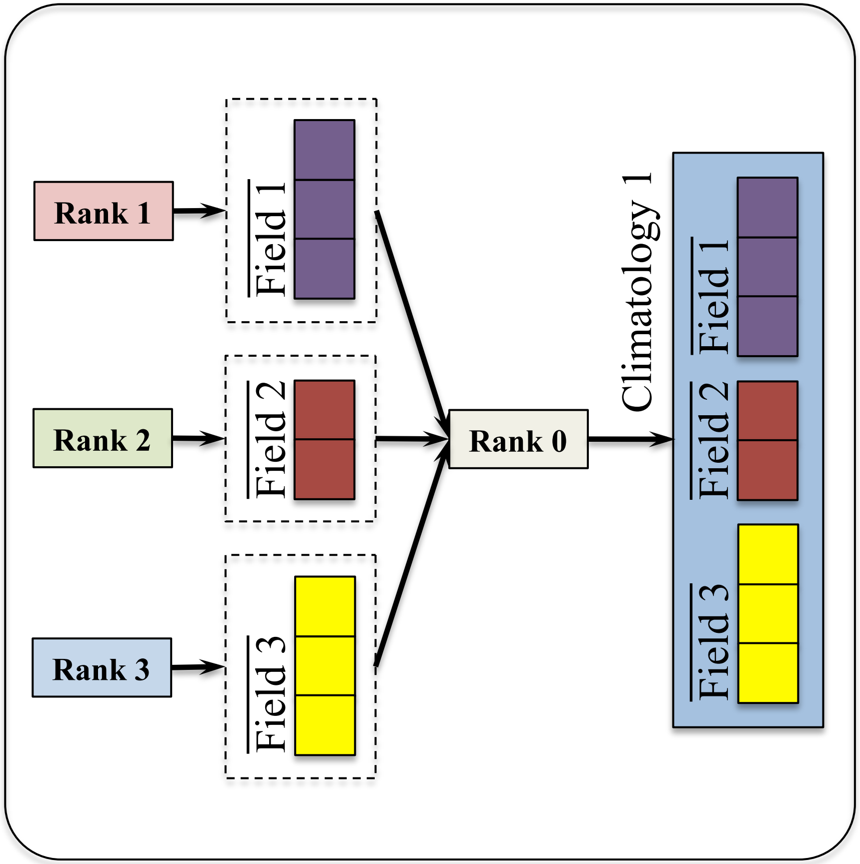


Task Parallelism

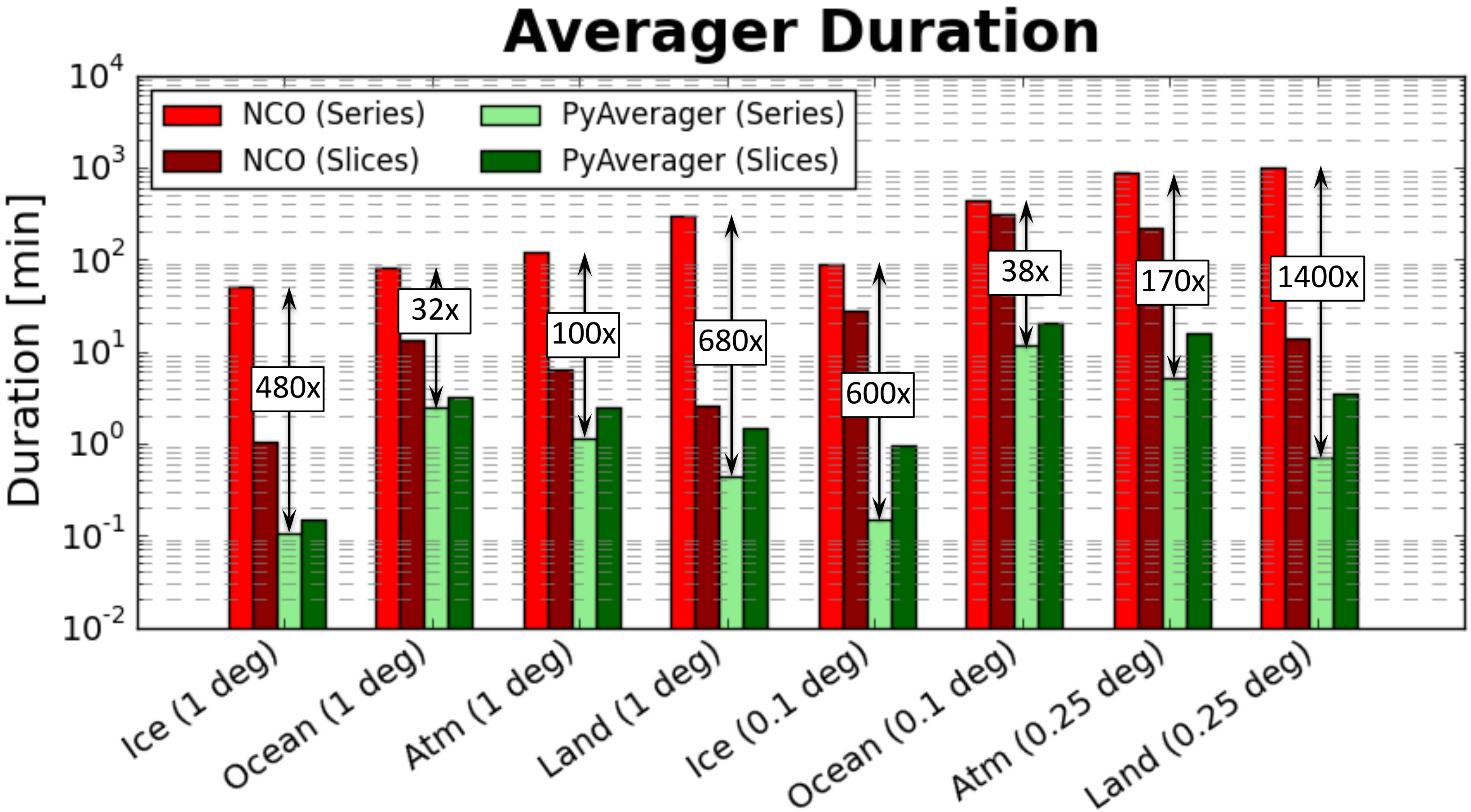


Task Parallelism

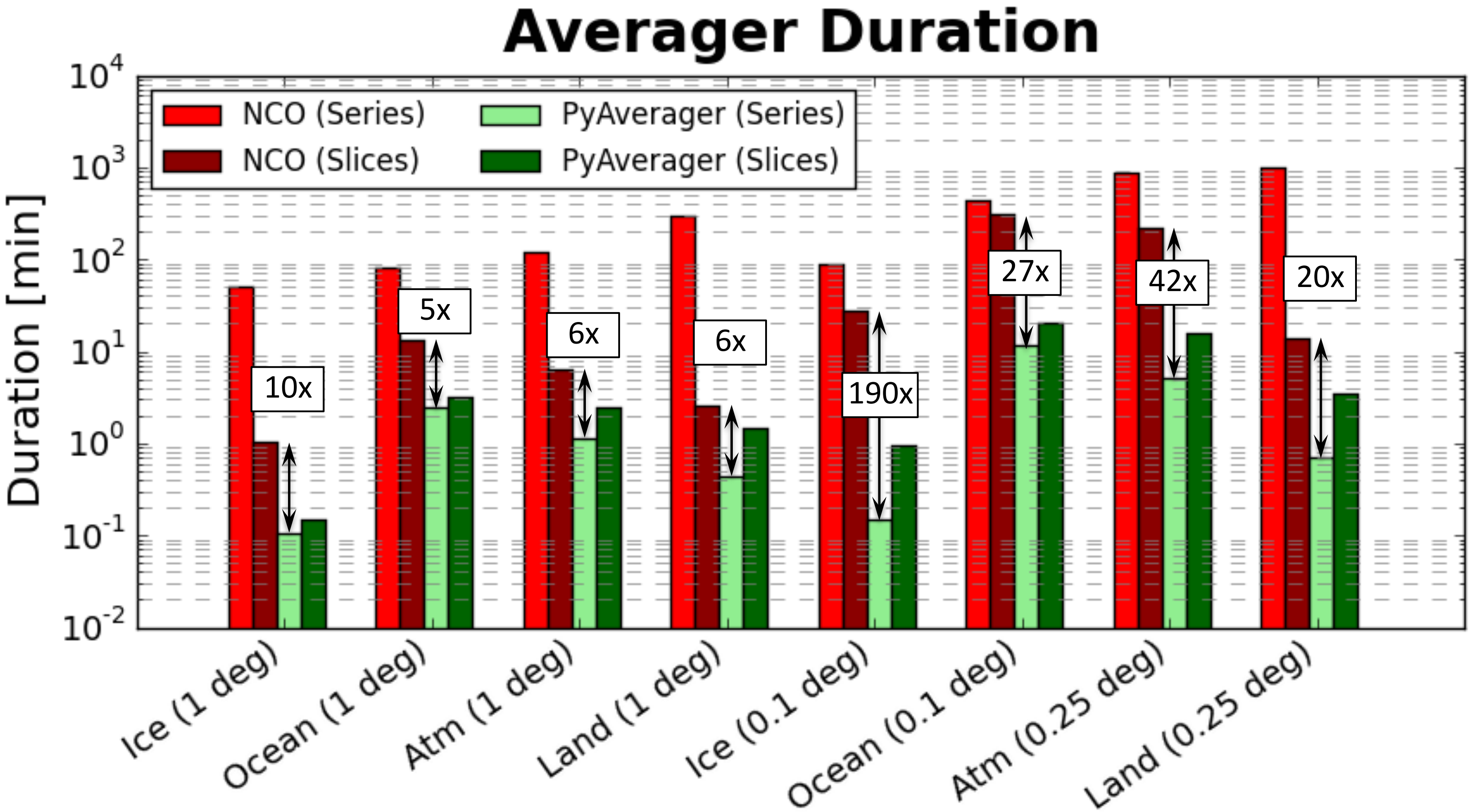
- Additional Parallelism over Climatologies
  - Seasons
  - Years
  - Months
- Climatologies Ordered:
  - Mos ➔ Seasons ➔ Yrs
- Each Climatology given its own MPI subcommunicator



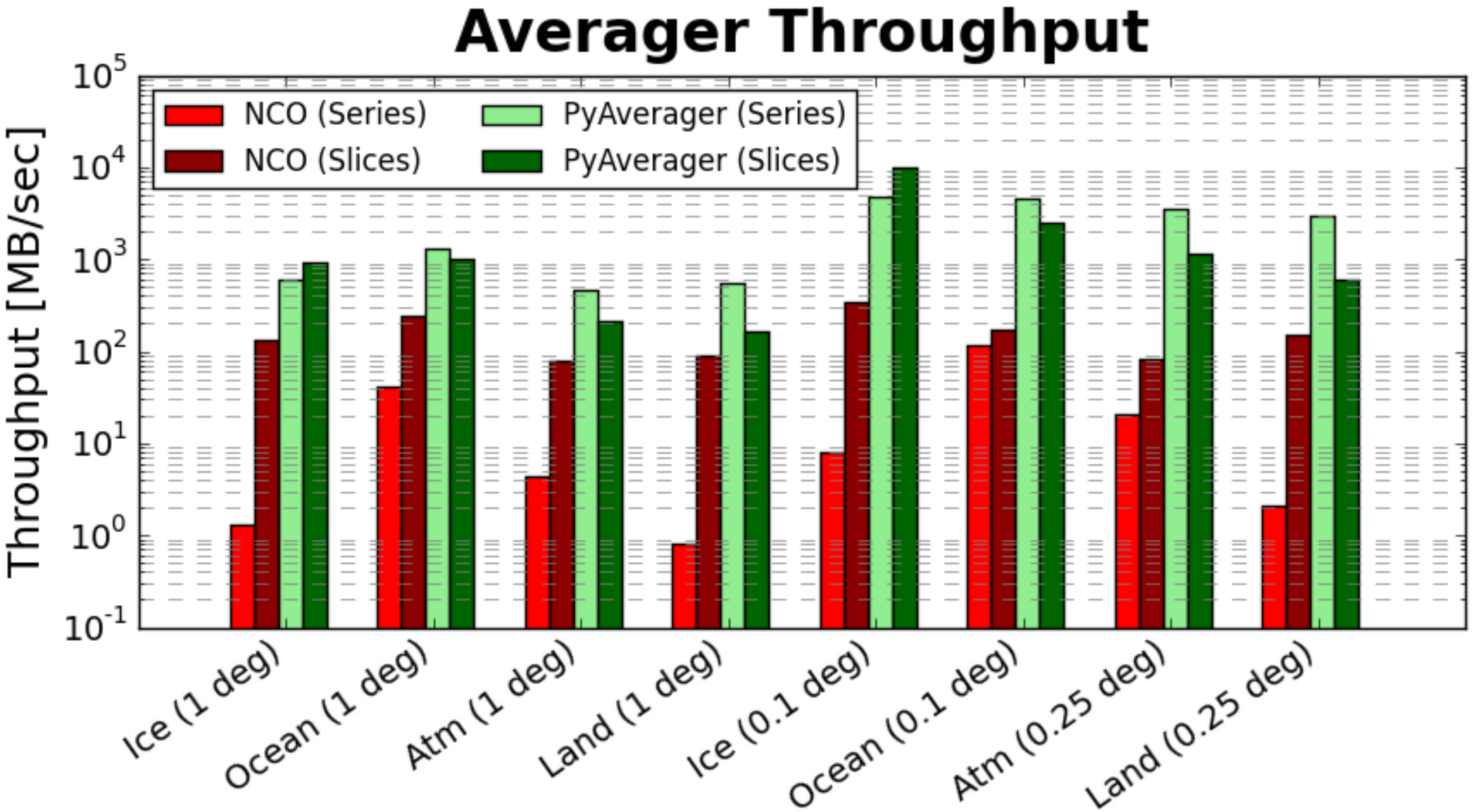
MPI Intercommunicator 1



- 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



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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/

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.