Community Diagnostics Package

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Introduction

- Framework for managing/modularizing tasks related to diagnostics
  - Handle using input
  - Computing metrics
  - Provenance capture
  - Running diags in parallel (multi-processing, distributedly)
- Basic structure but allows for independence, no dependencies
- Optional support for commonly used tasks
  - Graphing with VCS
  - Viewing results on a webpage created with the CDP viewer API
  - Metric calculations with CDAT (GenUtil, CdUtil)

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Problems Solved

- Scientific code is complex, so has a short life
- Scientists don't have the urgency to implement good software engineering principles
  - Should focus domain-specific work, not viewing results, parallelism, etc.
- Provides a framework for diagnostics to be shared
- Diagnostic packages built with CDP have similar architecture, easy for developers to transition across projects

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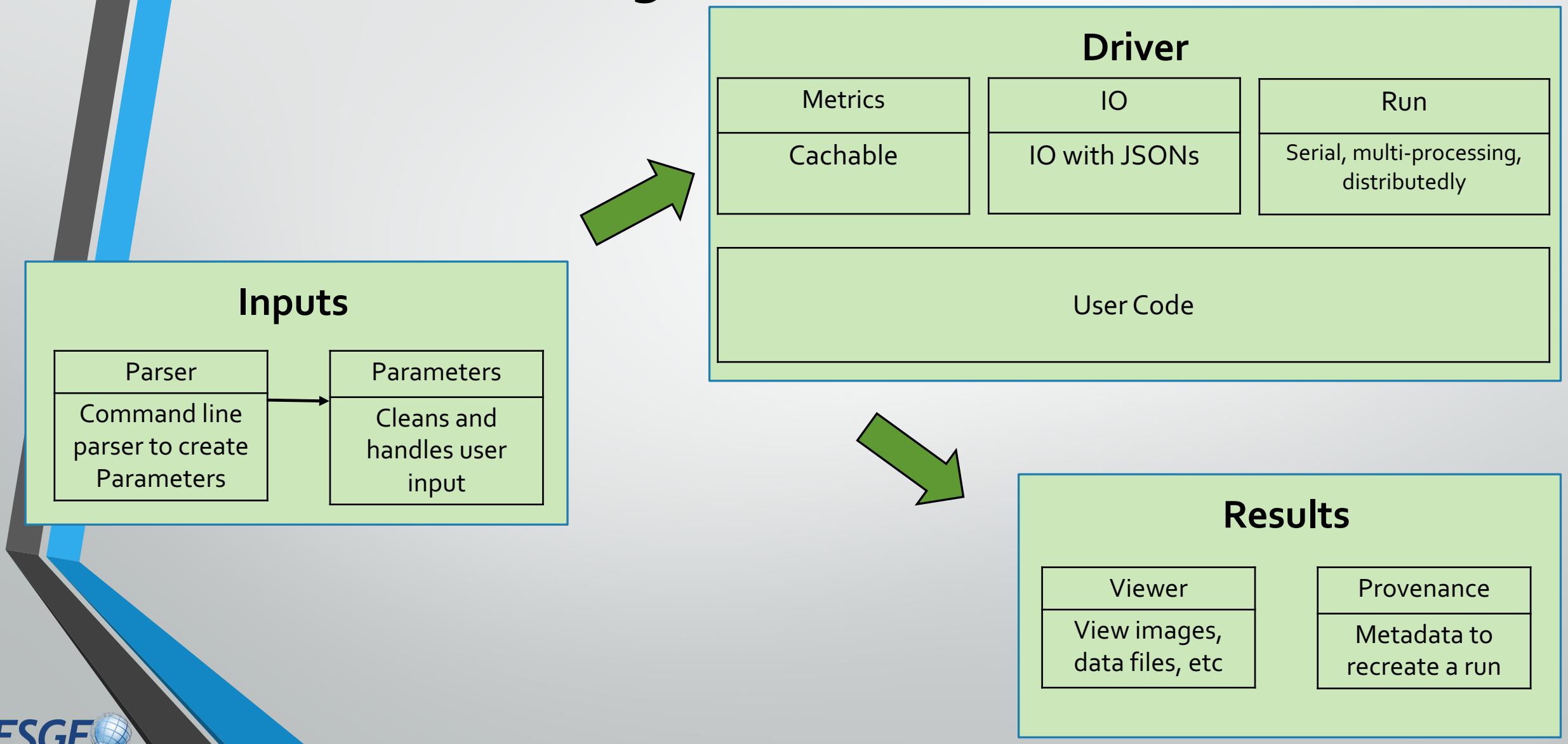
Design and Architecture



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Design and Architecture

- Parameters object:
  - Used as input, created from a Python script
  - Encapsulates sanitization of user input
- Parser object: creates Parameters object from the command line
  - Takes raw file: `diags_package.py` **`-p myparams.py`**
  - Individual parameters are command line arguments, ex: `diags_package.py -p myparams.py` **`--seasons ANN`**
- Example parameters script:

```
variables = ['T', 'PRECT']
regions = ['global']
seasons = ['ANN', 'DJF']
```

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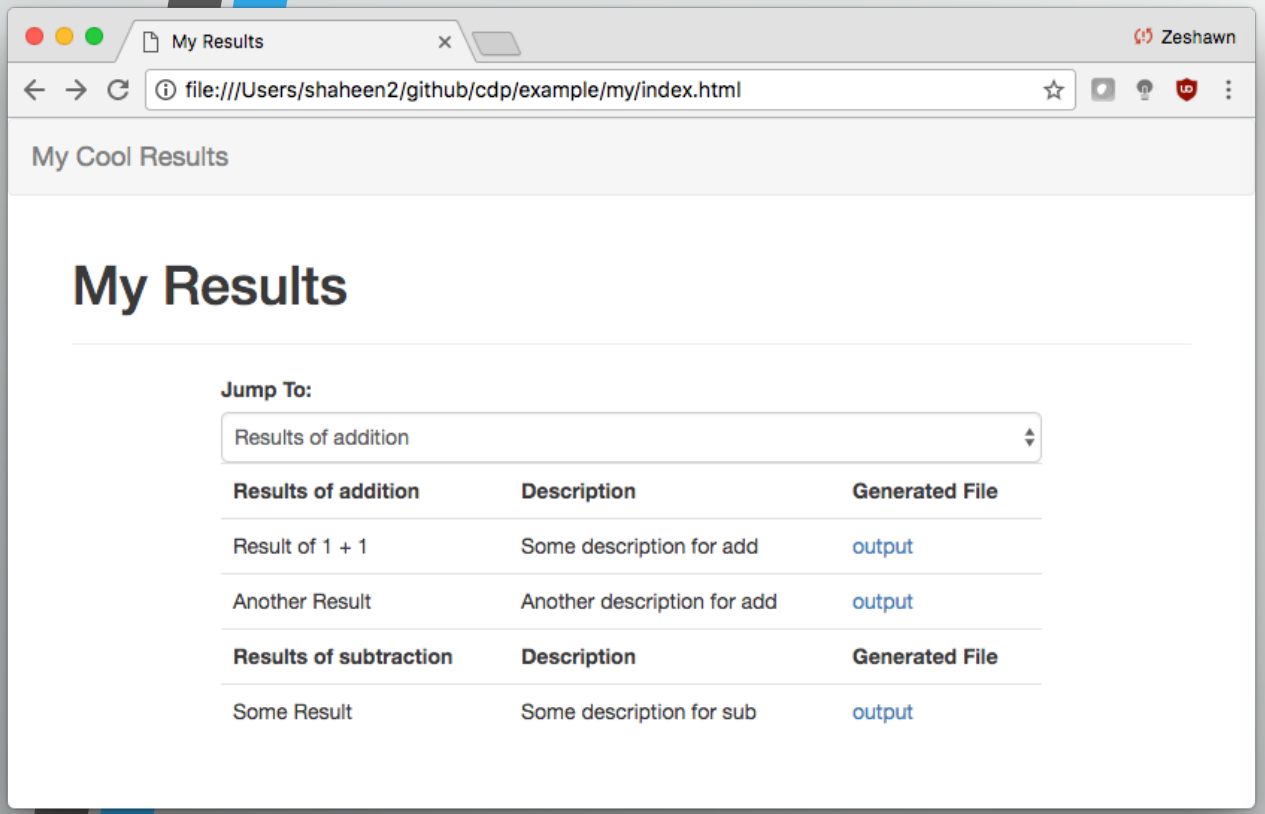
Design and Architecture

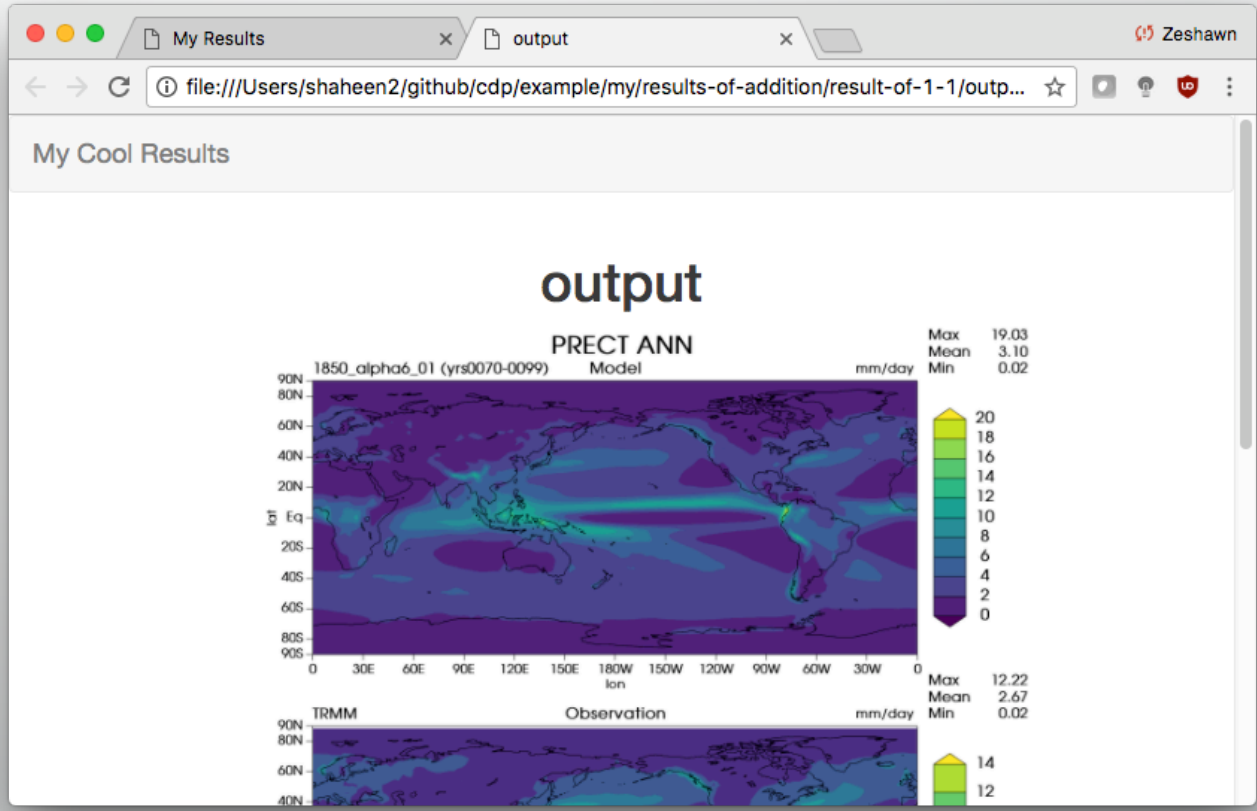
- Metrics:
  - Cachable, not in by default in Python 2
  - Single interface to work with Fortran, C, Python code
  - ESGF CWT-based metrics as well
- IO:
  - Handles input/output with JSONs
- Main script (driver), designed for a single run
  - Input: Parameters object
  - Do calculations using metrics, save info with IO, etc
  - Results: View results with CDP viewer, provenance capture through CDP provenance.

Design and Architecture

- Run:
  - Run a driver in serial, or parallel using multi-processing or with distributed computing
  - Data parallelism with different parameters
- Viewer:
  - Easily create an interactive, sharable HTML page
  - In Python, no HTML/Javascript
- Provenance:
  - Create a backup of the Parameters object
  - Log of output, utils for data validation (hashing, etc)

Design and Architecture





- Only 14 lines of code

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Design and Architecture

- Data parallelism
  - User can submit multiple runs:
    - `diags_package.py -p myparams1.py myparams2.py`
    - `diags_package.py -p myparams.cfg`
  - Compose parameters:
    - `diags_package.py -p myparams.py –d myparams.cfg`
  - **Transparency**:
    - Each run is a job
    - Same interface to run in serial, parallel, parallel w/ distributed
    - Users don’t need to tailor input to match the type of run
  - CDP CLI
    - Tool for viewing status of, restarting, killing distributed jobs

```
[diags1]
vars = ["T"]
seasons = ["ANN", "SON"]

[diags2]
vars = ["PRECT"]
seasons = ["JJA"]
```

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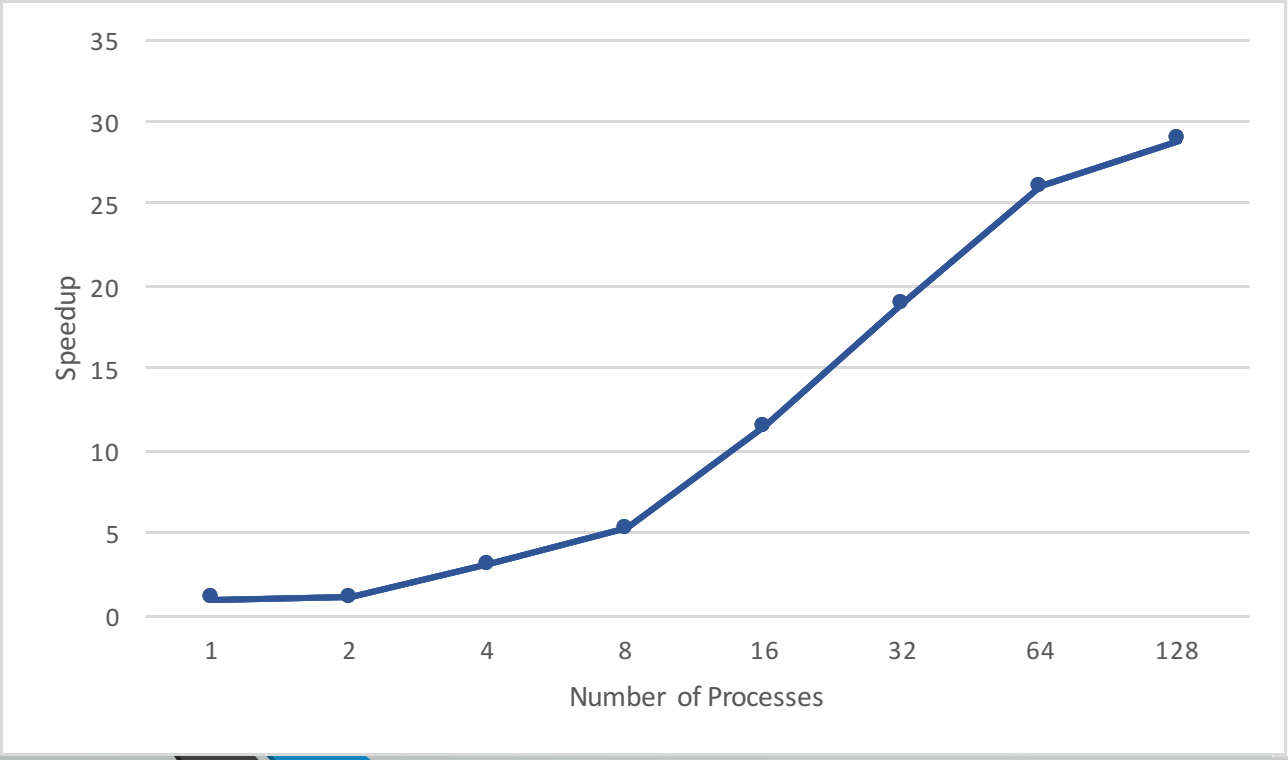
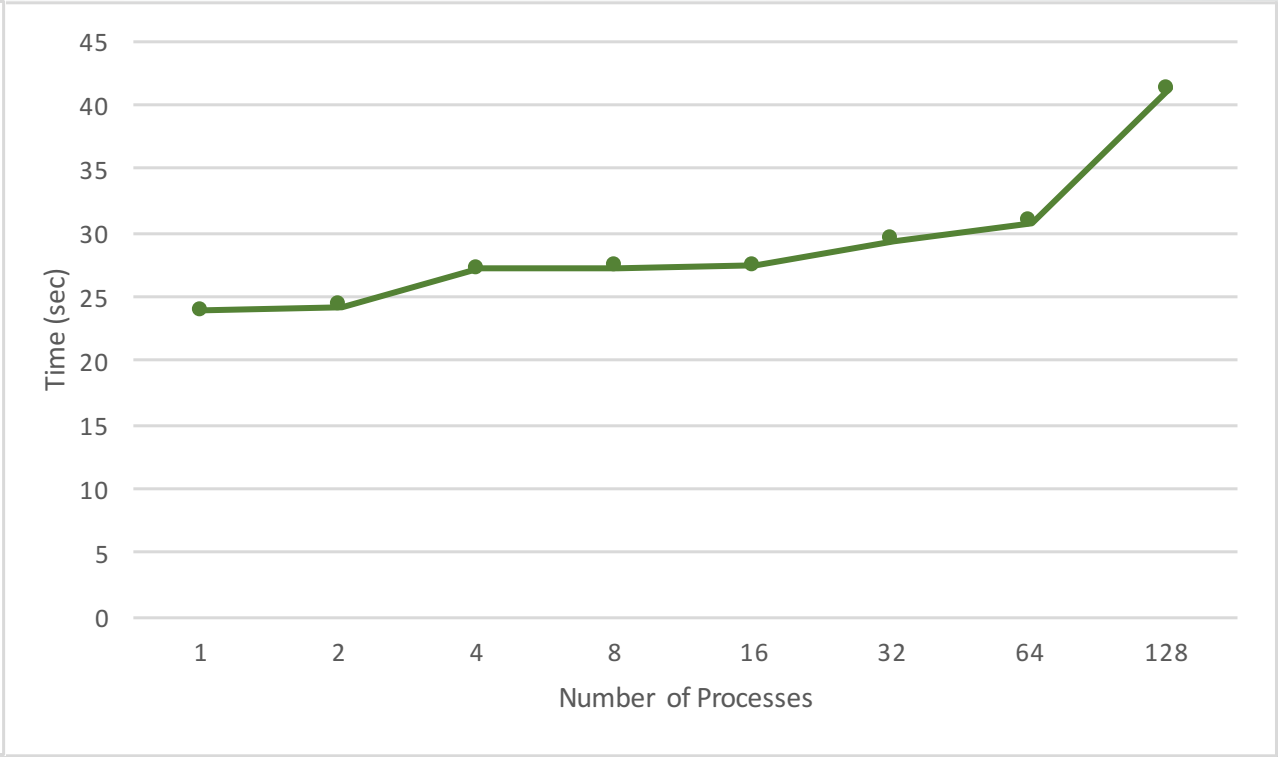
Design and Architecture

- E3SM Diagnostics Package performance, w/ 1330 individual diagnostics
- Good strong and weak scaling





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Uses

- PCMDI Metrics Package:
  - Completed January 2017
  - Need to add new features
- E3SM Diagnostics Package
  - In progress, 7 plot sets done
  - Replacement for AMWG Diagnostics
- ARM Diagnostics

Future Work

- Cloud computing
  - Containerize software, deploy on PaaS (AWS, Google Cloud Platform, etc)
- Library of metrics, but would introduce more dependencies
- Standardize more components
  - Ex: Interface for plotting reference, test, and diff data
    - `plot(reference, test, difference)`
- Finish implementing E3SM Diagnostics, ARM Diagnostics, expand on PCMDI Metrics Package

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