GFDL FMS

Bronx to Chaco Rewrite

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In memoriam

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Overview

- Intro to GFDL, FMS, FRE
- Climate modeling workflow achievements
- How we're approaching a workflow rewrite
- Challenges, lessons learned

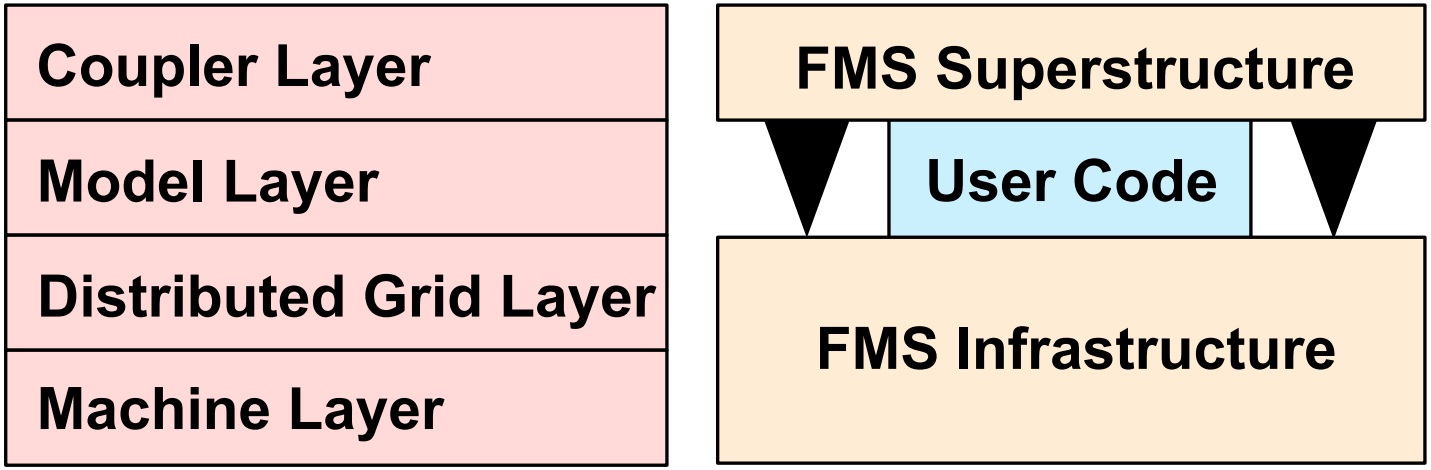
GFDL

Geophysical Fluid Dynamics Laboratory

- Mission: *To advance scientific understanding of climate and its natural and anthropogenic variations and impacts, and improve NOAA's predictive capabilities*
- Joint Institute with Princeton University
- About 300 people organized in groups and teams
  - 8 scientific groups
  - Technical Services
  - Modeling Services
    - Framework for coupled climate modeling (FMS)
    - Workflow software (FRE), Curator Database
    - Liaisons to scientific modeling efforts

Flexible Modeling System

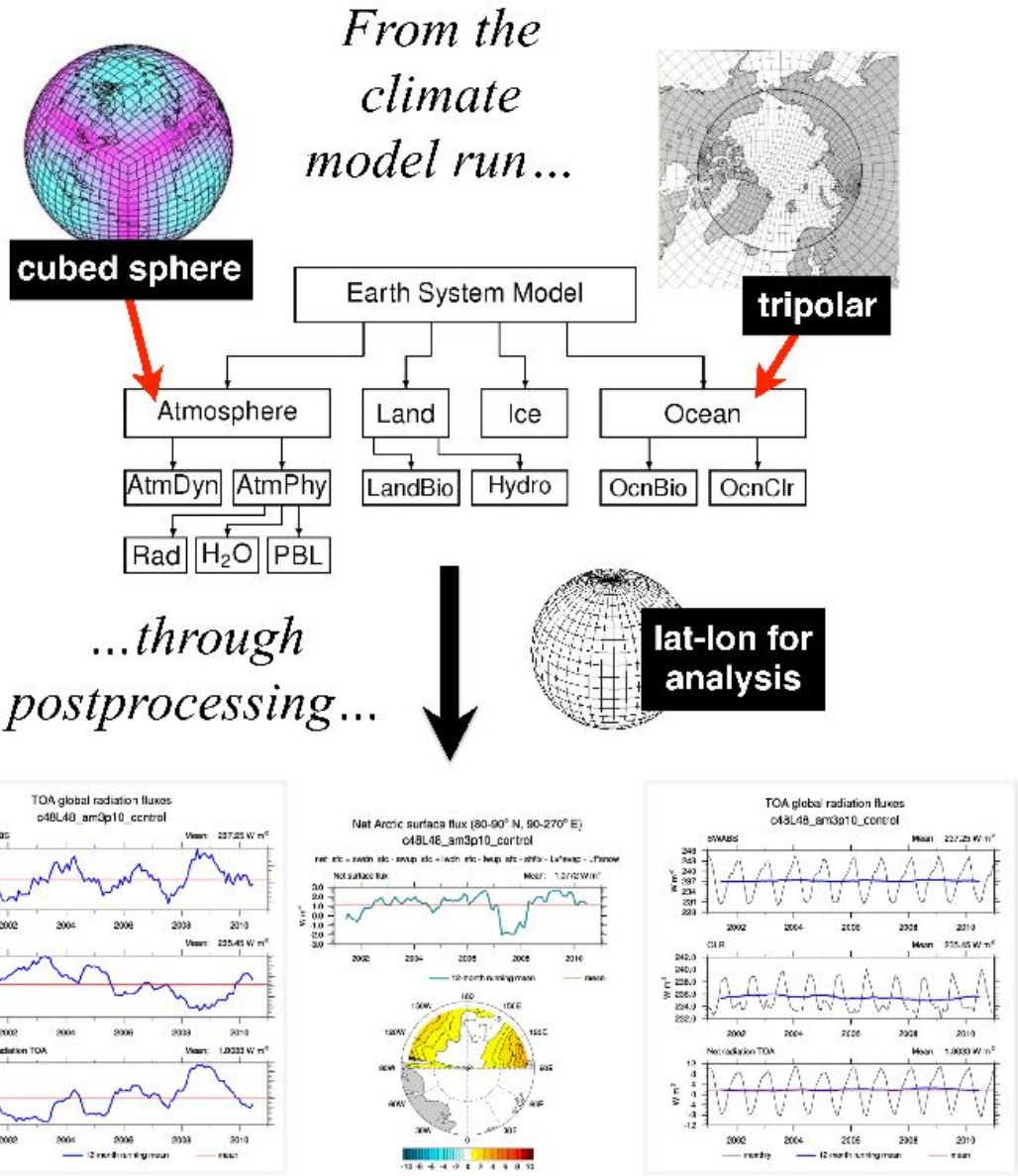
- FMS is a software framework which provides infrastructure and interfaces to component models and multi-component models.



- Started ~1998, development timelines:
  - Component models by scientific group, continuous
  - Annual FMS city releases, 200+ configurations tested

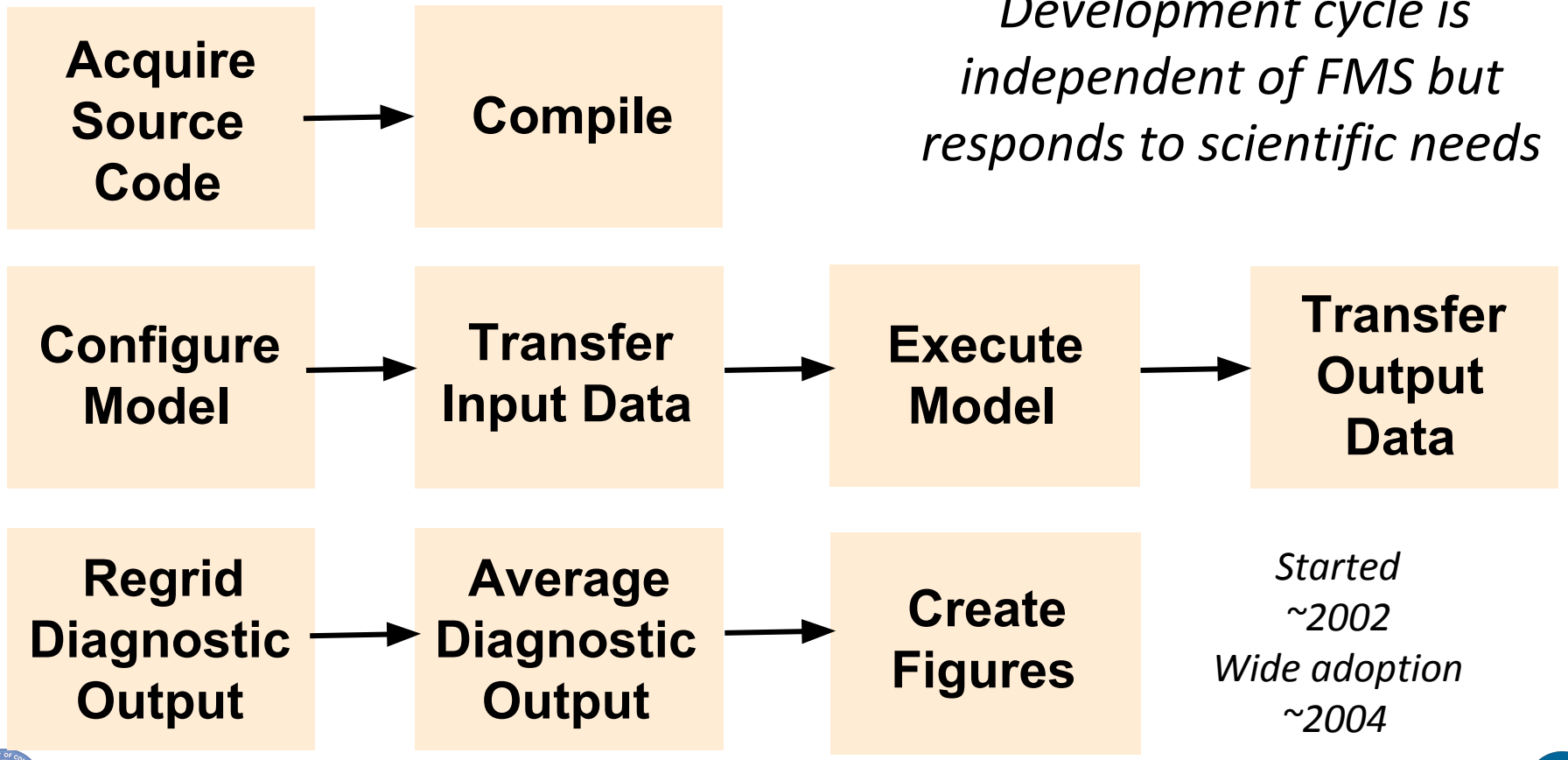
Workflow Goals

- Reproducibility
- Perturbations
- Differencing
- Robustness
- Efficiency
- Error handling: user level & system level



FMS Runtime Environment

FRE is a set of workflow management tools that read a model configuration file and take various actions.



Development cycle is independent of FMS but responds to scientific needs

Started ~2002
Wide adoption ~2004

FRE Technologies

- XML model configuration files, and schema
  - User and canonical XML
- Perl command line utilities read XML file
- Site configuration files
  - Script templates
  - Conventions for file names and locations
- Environment modules to manage FRE versions
- Moab / Torque to schedule jobs across sites
- Transfer tools: globus + local gcp, HSM tools
- NCO Operators + local fregrid, plevel, timavg
- Jenkins for automated testing
- *Coming soon: Cylc*

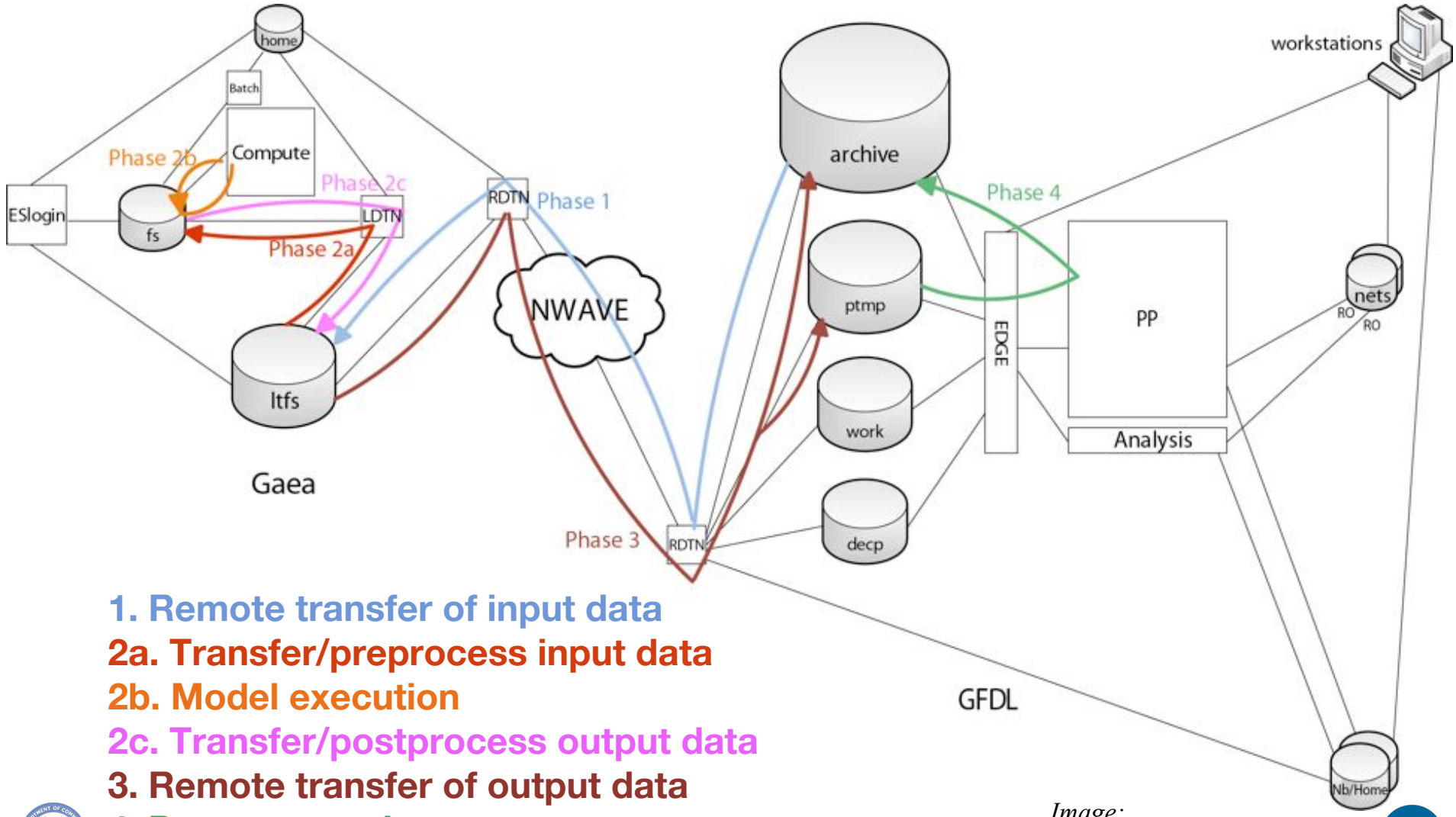
FRE Features

- Encapsulated support for multiple sites
  - Compiler, scheduler, paths, user defaults
- Model component-based organization of model configuration
- Integrated bitwise model testing
  - Restarts, scaling (vs. reference and self)
- Experiment inheritance for perturbations
- User code plug-ins
- Ensemble support
- Postprocessing and publishing, browsable curator database

FRE Job Stream Overview

- Experiments run in segments of model time
  - Segment length is user-defined
  - More than one segment per main compute job is possible
- After each segment:
  - State, restart, diagnostic data is saved
  - Model can be restarted (checkpointing)
  - Data is transferred to long term storage
  - A number of post-processing jobs may be launched, highly task parallel

Flow Through The Hardware



1. Remote transfer of input data
2a. Transfer/preprocess input data
2b. Model execution
2c. Transfer/postprocess output data
3. Remote transfer of output data
4. Post-processing

Image: Tara McQueen

GFDL Data Stats

- Networking capacity ORNL to GFDL: two 10gig pipes,120 TB/day theoretical for each pipe
- Analysis cluster:
  - ~100 hosts with 8 to 16 cores, 48GB to 512GB memory, local fast scratch disk of 9TB to 44TB
  - 4 PB/week throughput
- Tape-based data archive: 60PB
  - ~2PB disk attached
  - Another ~2PB filesystem shared among hosts for caching intermediate results
- 1300 auto-generated figures from atmos model
- An early configuration of CM2.6 (0.1 degree ocean, 0.5 degree atmos) runs on 19,000 cores
  - a year of simulation takes 14 hours and generates 2TB of data per simulation year, ran 300 simulation years

Post-processing Defined

- Preparing diagnostic output for analysis
  - Time series: Hourly, daily, monthly, seasonal, annual
  - Annual and Seasonal climatological averages
  - Horizontal interpolation: data on various grids can be regridded to lat-lon with “fregrid”
  - Vertical interpolation: to standard pressure levels
  - Hooks to call user scripts to create plots or perform further data manipulation
  - Enter the model into the curator database
- Requirement: must run faster than the model
- Self healing workflow: state is stored; tasks know their dependencies and resubmit as needed

10 Years Later...

Oh, the clusters you'll run on and the lessons you'll learn...

FMS FRE Chaco

- Rewrite of FRE begining with post processing
- Maintain compatibility and historical behavior, yet standardize tool behavior
  - Old (user) interfaces available, e.g. ‘drop in’ replacement where possible
- Improve visibility and control of experiments

Chaco Major Goals

- Robustness and reliability
- Support for high resolution resource requirements
  - CM2.6, a higher resolution model, generates 2TB per simulation year, completes 2 sim years/day
- Support for discrete toolset that can be used without running end to end “production frepp”
- Monitoring
- Increased task parallelism
- Maintain existing functionality
- Keep pace with data flow rate from remote computing sites (gaea/theia/titan…)

High Resolution Strategy

- Reduce memory and disk space requirements
- Initially break all diagnostic data up into “shards”
  - “Shard” files contain one month’s worth of data for one variable
  - Shards can be on model levels or regridded
  - Perform data manipulations on one variable at a time, then combine data later if necessary
  - Operations on shards can be highly parallelized
- Make intelligent use of disk cache with intermediate data
- Reducing data movement is key
  - Overwhelming majority of the time spent in postprocessing is simply moving data

Black box to discrete toolset

Postprocessing

- Outside looks the same

```
frepp -v -c split -s -D  -x FILE.XML -P
SITE.PLATFORM-COMPILER -T TARGET-STYLE -d
MODEL_DATA_DIRECTORY -t START_TIME EXPERIMENT_NAME
```

- Inside nothing is the same

FRE Utilities

Bronx		*Chaco*
`fremake`	obtain code, create/submit compile scripts	
`frerun`	create and submit run scripts	`fre cylc run`
`frepp`	create and submit post-processing scripts	`fre cylc prepare`
`frelist`	list info about experiments in an xml file	`fre list`
`frestatus`	show status of batch compiles and runs	`fre monitor`
`frecheck`	compare regression test runs	
`frepriority`	change batch queue information	
`freppcheck`	report missing post-processing files	
`frescrub`	delete redundant post-processing files	
`fredb`	interact with Curator Database	

Bronx Design

- Bronx implementation: monolithic, linear perl script re-invoking itself over subsequent segments of model data. Steps to produce desired products hardcoded in blocks of shell which are assembled and submitted to batch scheduler.

Chaco Design, 1

- Discrete tools in a unified code base: data movement, refinement, interpolation, timeseries and timeaverage

```
fre data {get, split, zinterp,
xyinterp, refineDiag, analysis,
timeaverage, timeseries}
```

- Cylc-based cycle for experiment duration and model segments
- Per-cycle tool runs

Chaco Cylc

- Cylc for the dependency and scheduling engine
- Cylc suites generated by FRE Chaco
  - Allows for different grouping of tasks based on arguments, XML, or other factors.
  - User accessible / modifiable, but ‘hidden’
- Leverage Cylc task management and job submission
- Cylc GUI gives visibility and control

Chaco Design, 2

- Segments run in parallel:
  - Multiple MOAB jobs on separate nodes
- Tool commands
  - Utilize FRED to store parsed XML, diagfield info
  - Run concurrently over model components and model variables (shards)
  - Log all stdout, stderr, cpu, memory utilization, execution time

Chaco Tool Outline

- Modularize the monolithic workflow
- Standardize interface
  - ‘fre CATEGORY ACTION [OPTIONS]’
- Can operate independent of workflow
- On-disk data structure (FRED) stashes parsed experiment details
- File inventory and tool run databases
- Tools know input and output files

Chaco Tech

ENGILITY
Engineered to Make a Difference

- Perl OO via Moose and friends
  - Path to Perl 6
- CPAN all things
- Test driven development with continuous integration tactics.
- Strong source code practices, code documentation and project management tools to enable the team.

FRE PostProcessing, 1

- **Get, Split, and Stage**
  Retrieve data from storage, separate into variable shards, copy to shared temp filesystem.
- **Interpolate in Z, and XY**
  Stage shards in, interpolate, stage out
- **Generate Timeseries**
  Stage shards in, timeseries, store product
- **Generate Timeaverage**
  Stage shards in, timeseries, store product

FRE PostProcessing, 2

Reality check!

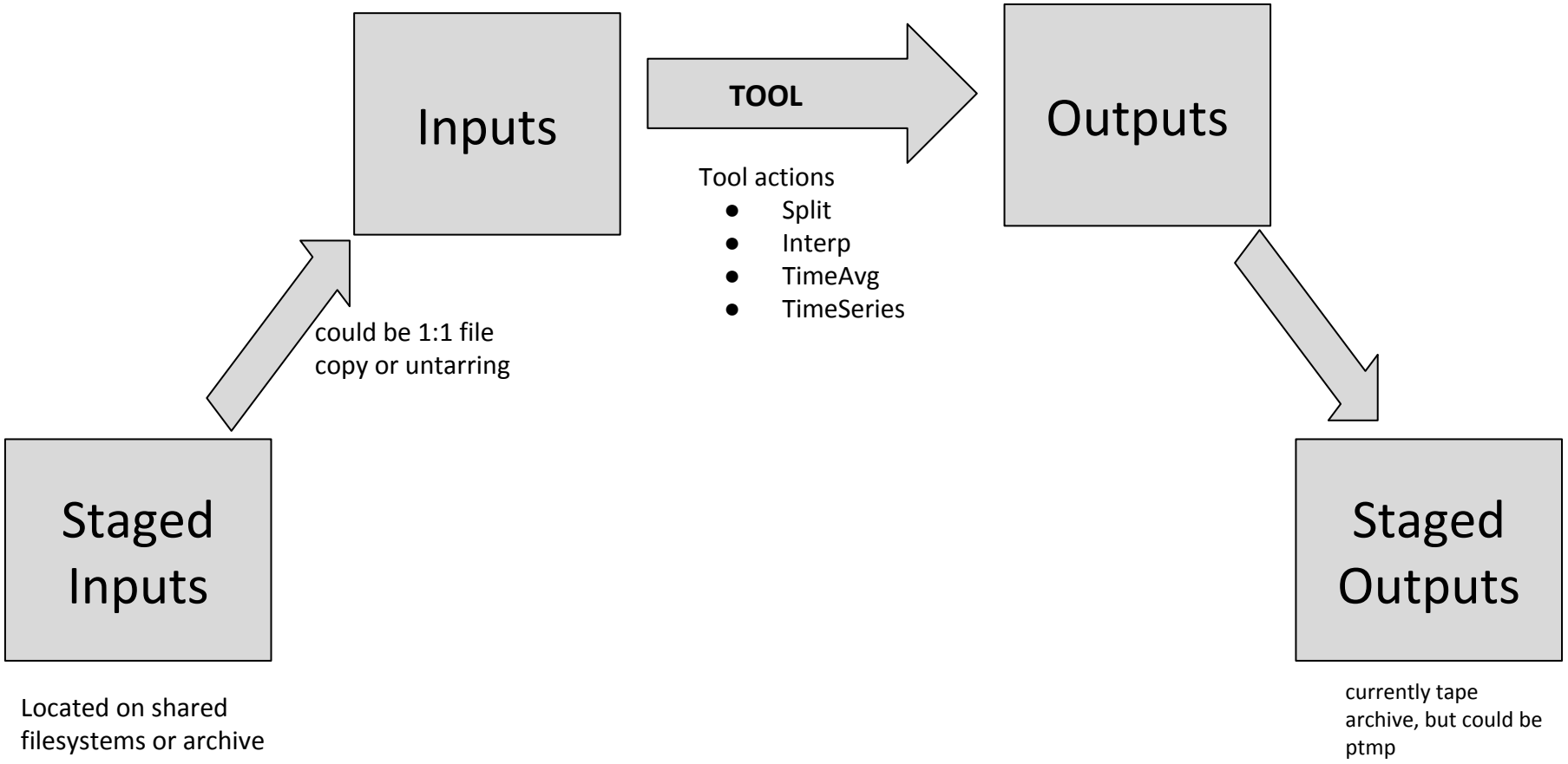
- **Get, "RefineDiag", Split, and Stage**
  Retrieve data from storage, run user-specified scripts to "refine data", separate into variable shards, copy to shared temp filesystem.
- **Interpolate in Z, and XY**
  Stage shards in, interpolate, stage out
- **Generate Timeseries, timeaverage**
  Stage shards in, timeseries / timeavg, store product
- **"Analysis"**
  Run user-specified scripts to generate figures, etc

FRE PostProcessing, 3

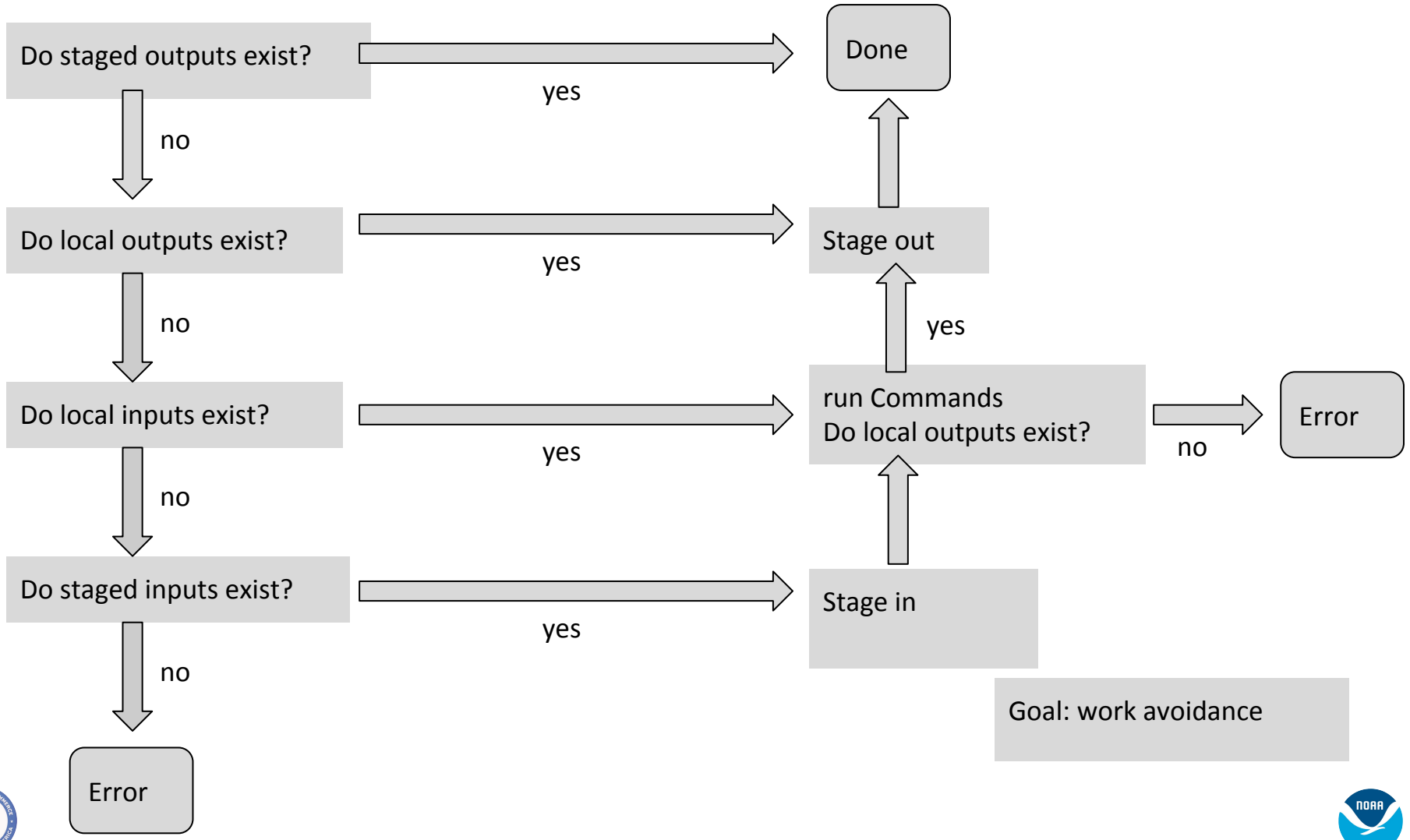
Dependency and Recovery check!

- Add knowledge of inputs and outputs to tools
- A Tool Operation framework for recovery and dependency-checking
  - Check for output (in final and local locations)
  - Check for inputs (in local and staged locations)
  - Run tool

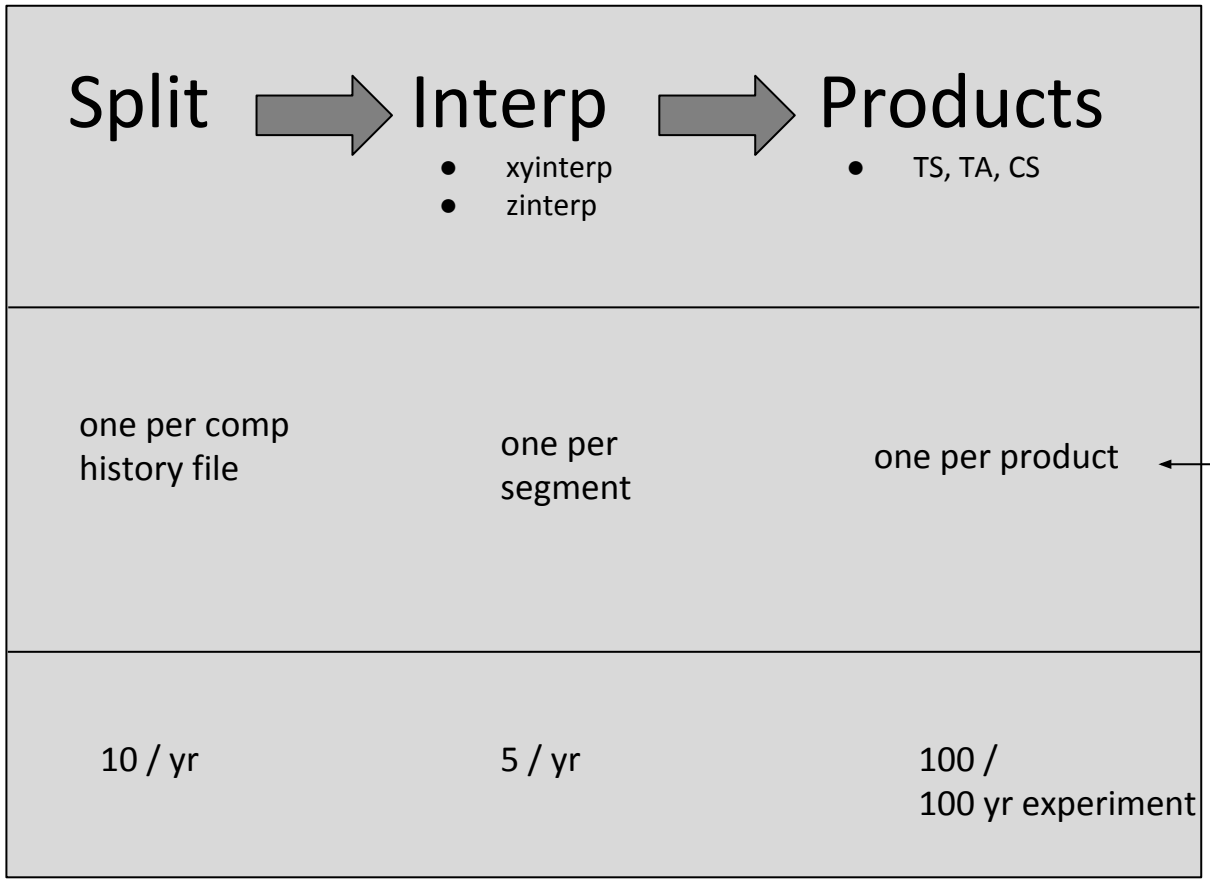
FRE Operation



Running an Operation



Operation Granularity



requests in XML (examples)

- 5 yr monthly TS ocean regridded to 1 deg
- All statics from land
- 10 yr seasonal TA atmos tracer native grid

Goals

- maximize outer-parallel
- make each be able to be a Cylc task without performance cost
- work avoidance

Tiers of concurrency

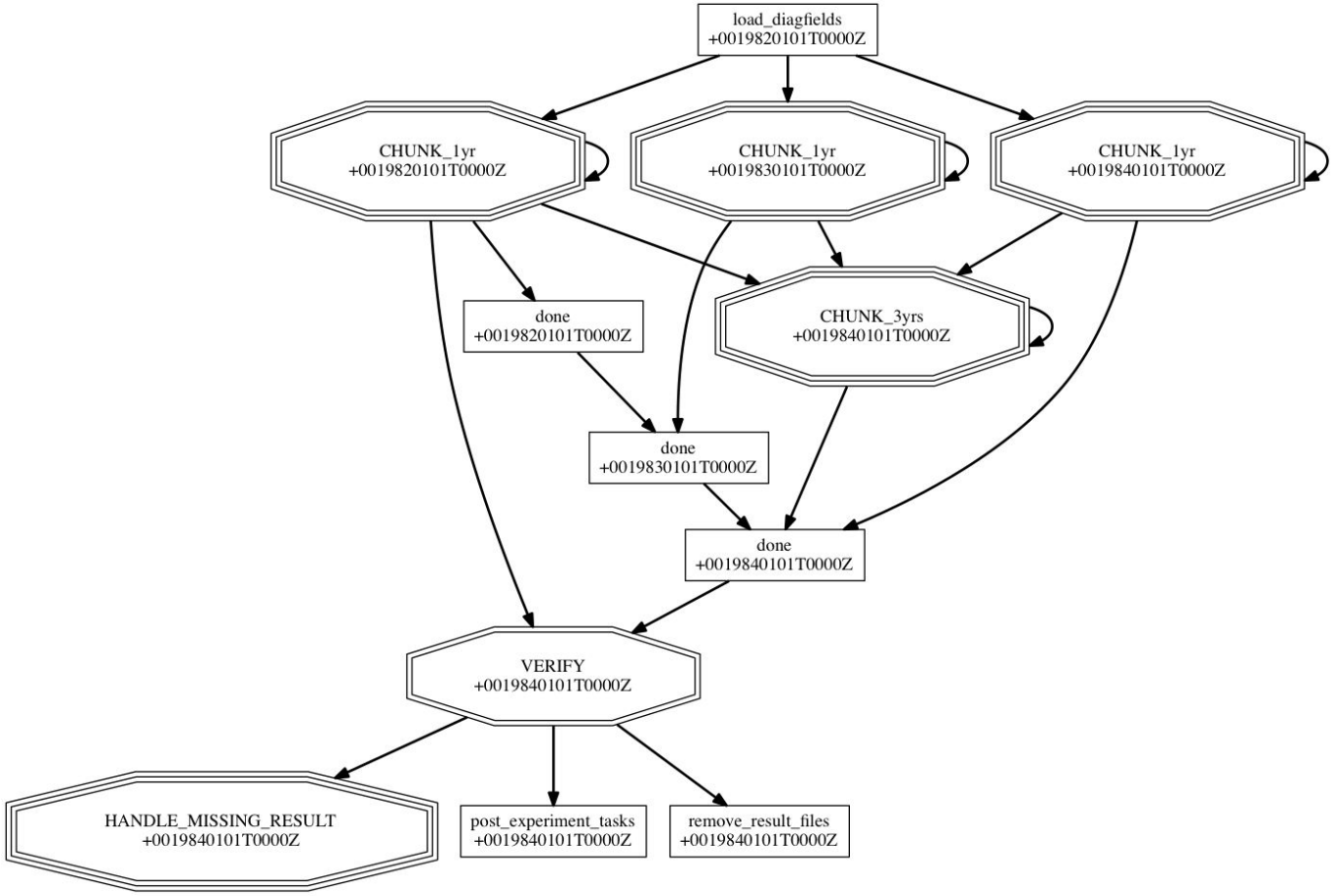
Goal: maximize inner-parallel by using tiers to isolate dependent commands

Example: One operation to create one annual timeaverage file containing all variables

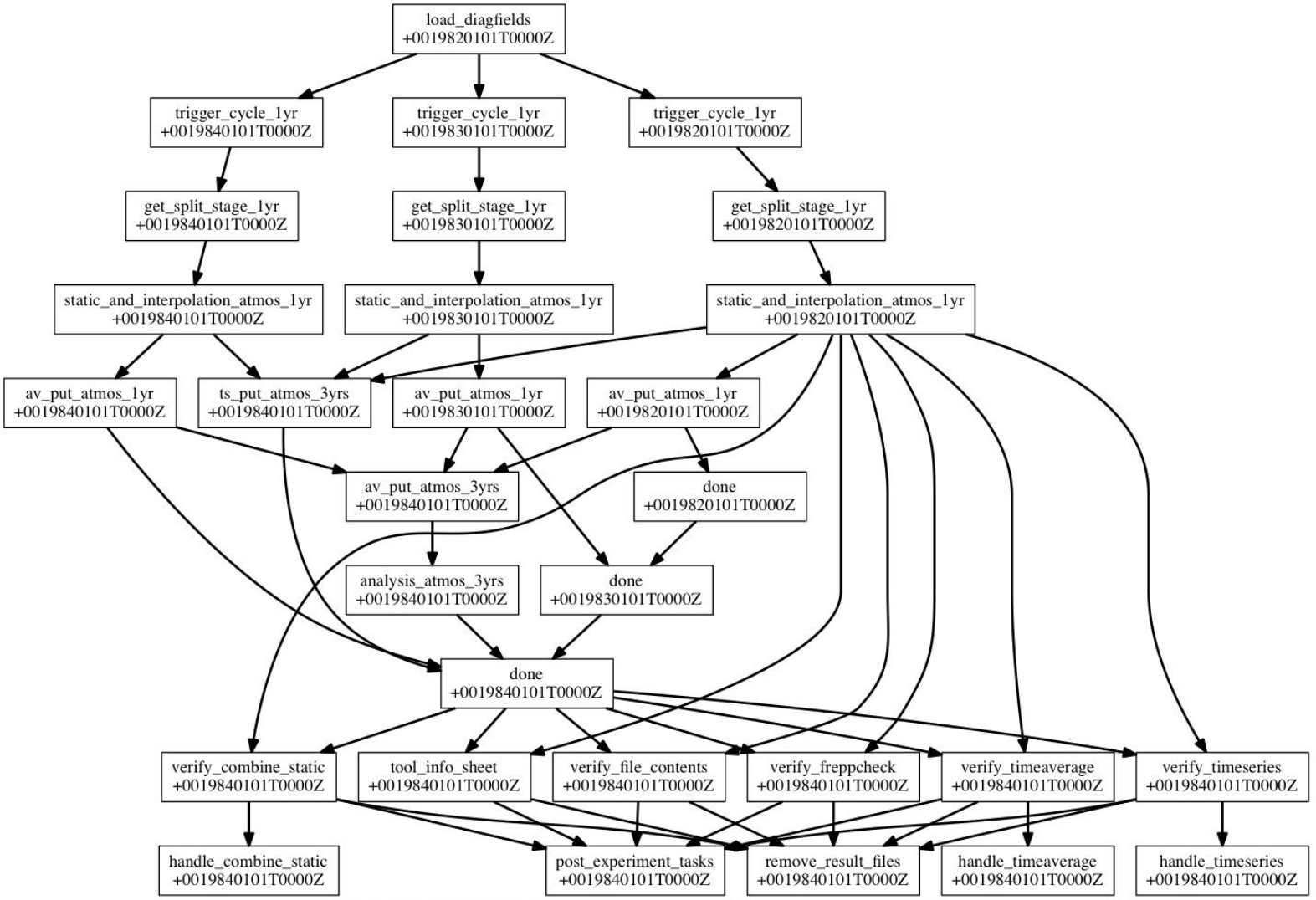
	Action	Tool	Parallelization
Tier 1	Concatenate shards to create TS	ncrcat	Number of variables
Tier 2	Average over TS timesteps	timavg (FRE tool)	Number of variables
Tier 3	Combine per-variable TA files into single file	ncks	1

FRE Workflow, 3yr test

3 year test and verify experiment

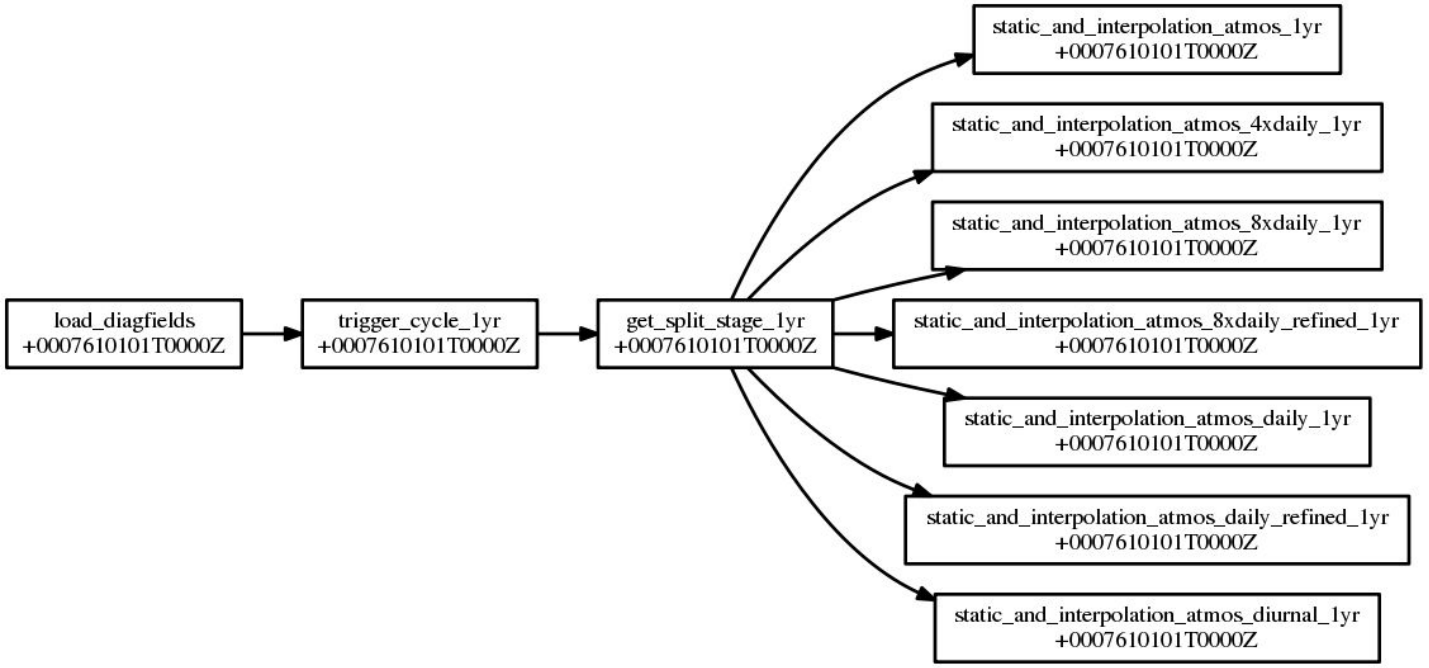


FRE Workflow, 3yr test



FRE Workflows

Simplified 1yr cycle of 100yr experiment



fre.verona.SM2_Control-1990.multiple.07610101-08600101

Current Status

- Alpha release available: *module load fre/chaco-alpha*
  - Have achieved full functionality for “quickstart” AM2, simplified c48 AM3, ESM2G, OM4, AWG
  - Differences in netcdf output vs. bronx exist but are understood
  - Workflow recovery dependency analysis
  - refineDiag: Create custom variables between run and postprocessing
  - Performance test performed; results currently under review
- Current work includes:
  - Adding ability to run in production from Bronx runscript
  - Review of performance data
  - Evaluate concurrency and parallelism
  - Adding experiment configurations to our test suite

Cool! So all the workflow issues are solved! Right??

When is the workflow broken?

- As complexity increases, a smaller and smaller percentage of error is tolerable
  - If 1% of jobs fail and your workflow launches thousands of jobs, you still have lots of work

- Our strategy: standard logging, retries, recovery, error handling, Cylc, automated test infrastructure in Jenkins…

Analyzing Chaco 1

- Analyze timing and resource metrics

  Performance Analysis of Chaco
- Tracking details at many levels
  - Individual commands (ncks, gcp)
  - Tiers of commands (run concurrently)
  - Command groupings
  - Segment runs
  - Tool runs

Analyzing Chaco 2

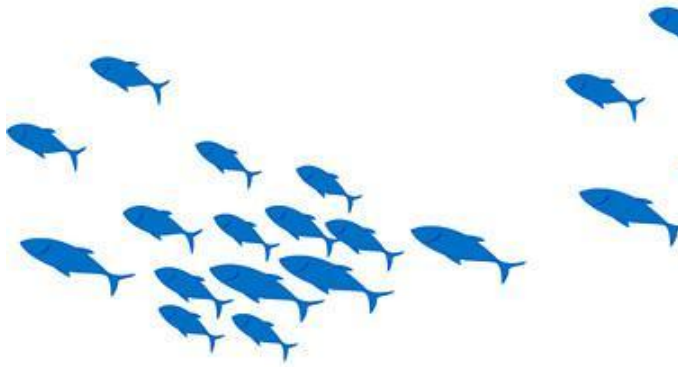
- What can we determine?
  - Variability
  - Data movement costs
  - Resource usage
- Areas under investigation
  - Per-node concurrency
  - Coalescing tasks

Pros and cons: user scripts

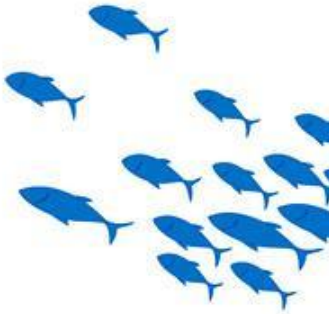
- Users can plug in shell scripting in several places
  - In runscript, before & after postprocessing
- Enables scientific exploration
- Enables great flexibility within FRE
- Often terrible for the workflow, if best practices are not followed
- Error catching/handling is difficult

Aiming for disk affinity

- Data movement can be reduced if jobs that will reuse the same source data are launched on the same host with data in the attached local disk
- Implemented to a small degree in FRE, as a high-res option
- Must tune task parallelism vs. reduced transfers
- Difficult batch scheduling task to load balance the system



job schooling

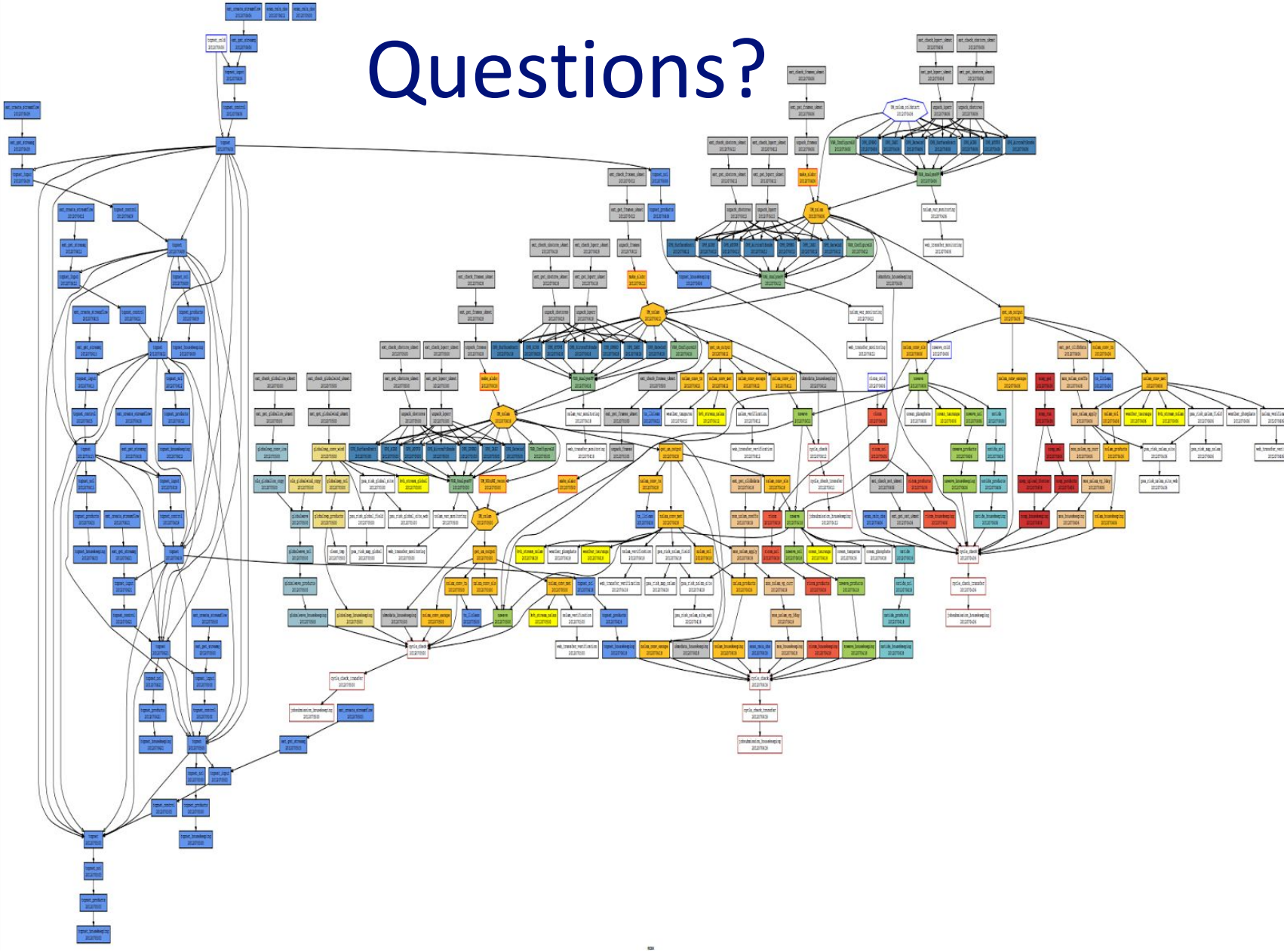


Art by zazerkale, redbubble.com

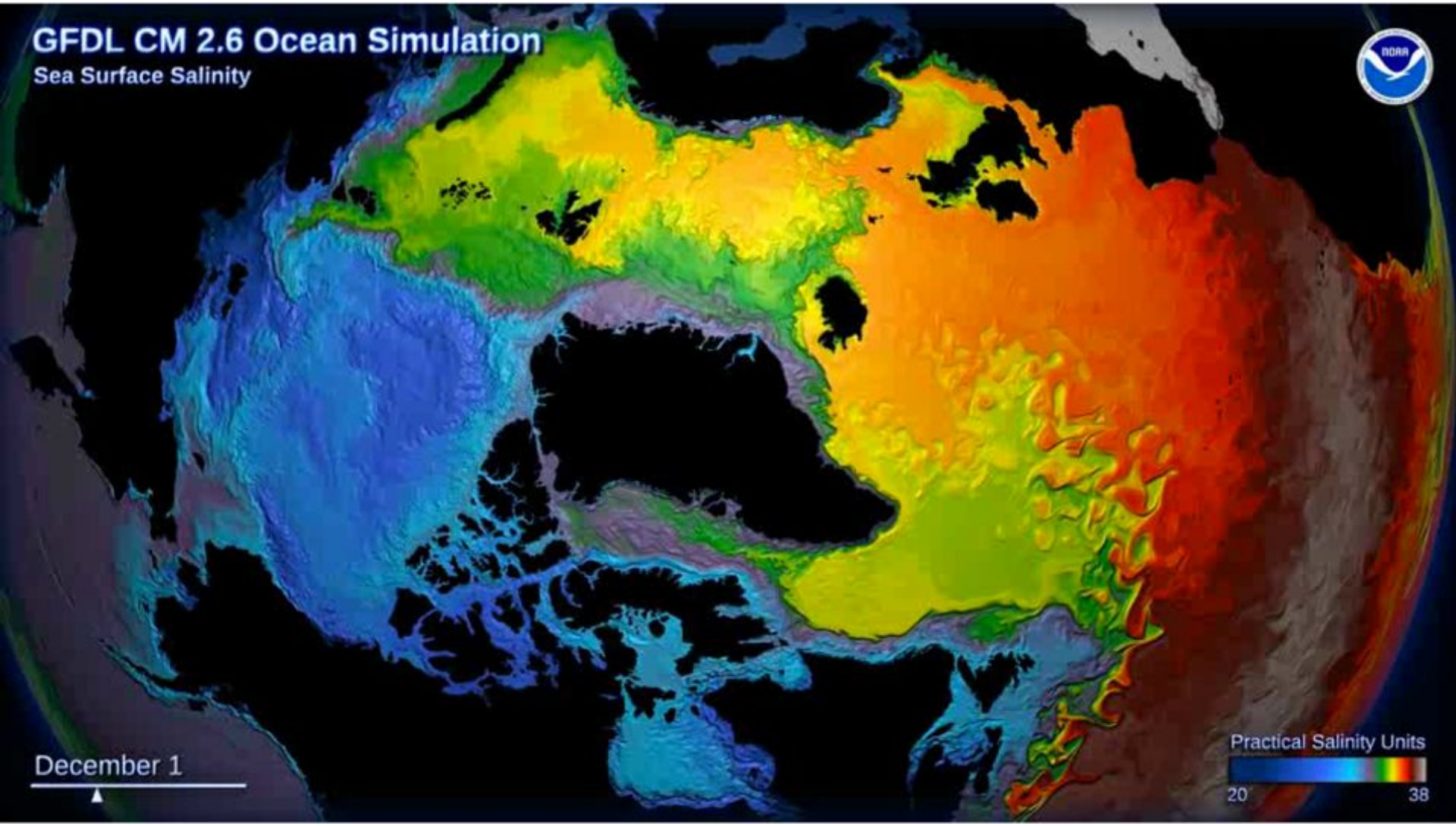
Workflow Discussion Points

- How can we reduce data movement?
- How much disk affinity can we achieve?
- Robustness: can we detect / recover from new error modes?
- How can we better leverage each other's work?
  - Automation vs. HPC security concerns
- How can we manage user plug-ins to the workflow?
- Do you trust your state files or check the filesystem?
- How do we handle user changes during a run?

Questions?



Answers?


GFDL CM 2.6 Ocean Simulation
Sea Surface Salinity
December 1
Practical Salinity Units
20
38

Sample XML: Setup

```
<experimentSuite>
  <setup>
    <platform name=”gfdl.default”>
      <directory stem=”subdirectory/paths”/>
      <csh>
        module load intel
        module load fre
      </csh>
      <property name="FMS_ARCHIVE_ROOT"
                value="/archive/fms"/>
    </platform>
  </setup>
  <experiment name=””> ...
```

Sample XML: Experiment

```
<experiment name="CM2.5A_2" inherit="CM2.5">
  <component name="fms">
    <source vc="cvs" root="/home/fms/cvs">
      <codeBase version="riga">shared</codeBase>
      <csh>
        cvs up -r riga_arl shared/.../file
      </csh>
    </source>
    <compile>
      <cppDefs> -Duse_netCDF </cppDefs>
    </compile>
  </component>
  <component name="mom4p1"> ...
```

Sample XML: Input

```
<input>
  <namelist name="vert_diff_driver_nml">
    do_conserve_energy = .true.
  </namelist>
  <dataFile label="input" target="INPUT/"
            chksum="" size="" timestamp="">
    $(FMS_ARCHIVE_ROOT)/am2/cover_type_field
  </dataFile>
  <diagTable>
     diagnostic variable table
  </diagTable>
</input>
```

Sample XML: Runs and Jobs

```
<runtime>
  <production simTime="26" units="years"
              npes="120" runTime="12:00:00">
    <segment simTime="12" units="months"
             runTime="06:00:00"/>
  </production>
  <regression name="basic">
    <run days="8" npes="60" runTime="00:15:00">
  </regression>
  <dataFile label="reference">
    $(FMS_ARCHIVE_ROOT)/am2/riga/19950108.tar
  </dataFile>
</runtime>
```

Sample XML: Postprocessing

```
<postProcess>
  <component type="atmos" source="atmos_month"
       sourceGrid="atmos-cubedsphere"
       xyInterp="90,144" zInterp="era40">
    <timeSeries freq="monthly"
                chunkLength="5yr">
      <variables> precip, temp </variables>
      <analysis script="/home/template.csh"/>
    </timeSeries>
    <timeAverage source="monthly"
                 interval="5yr"/>
  </component>
</postProcess>
```

Archived Output

```
/archive/$USER/fre/CM2.1U_Control-1990_E1.M_3A
|-- ascii
|-- restart
|-- history
`-- pp
    |-- atmos
    |   |-- ts
    |   |   `-- monthly
    |   |       `-- 5yr
    |   |           |-- atmos.000101-000512.precip.nc
    |   |           `-- atmos.000601-001012.temp.nc
    |   `-- av
    |       `-- monthly_5yr
    |           |-- atmos.0001-0005.01.nc
    |           |-- atmos.0001-0005.02.nc
    …           …
```