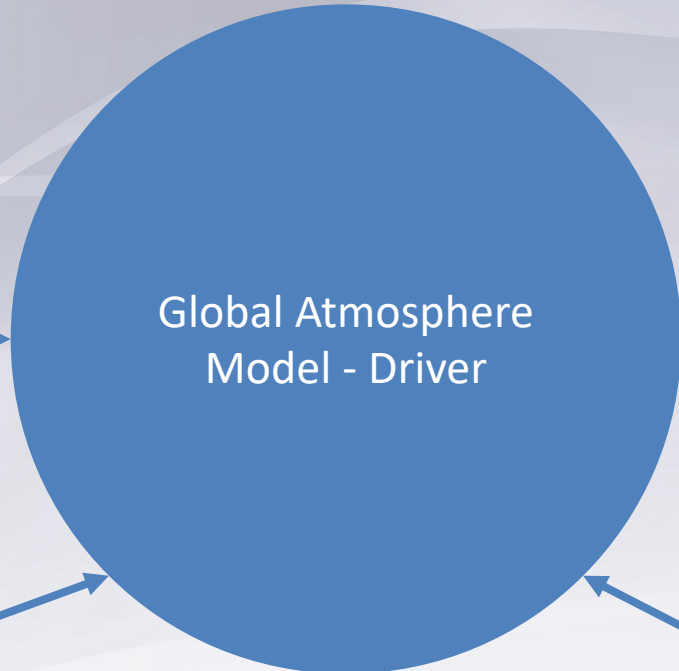




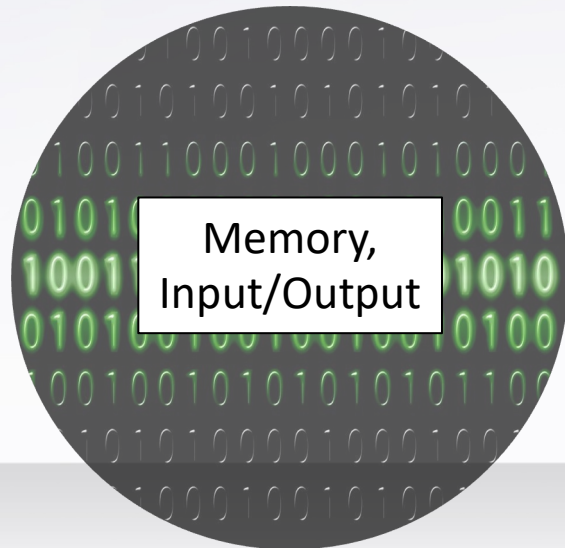
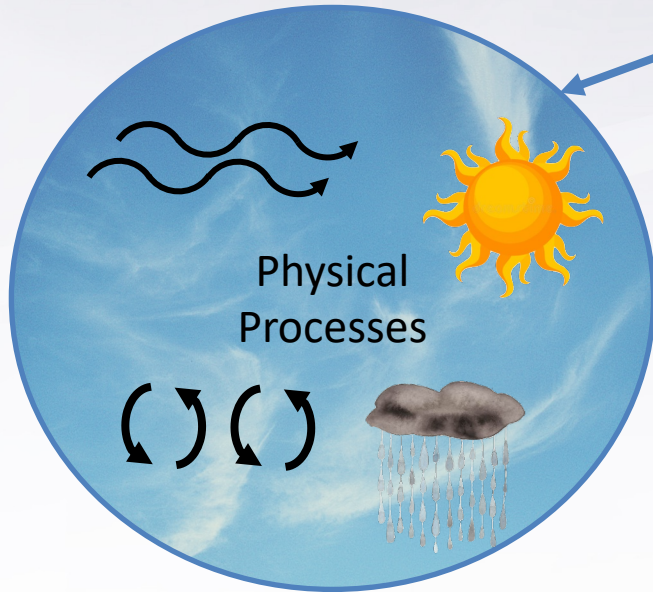
SCREAM – Designing a next generation global atmosphere model for exascale

Aaron S. Donahue*
CESM Workshop 2024
June 11, 2024

*and many more

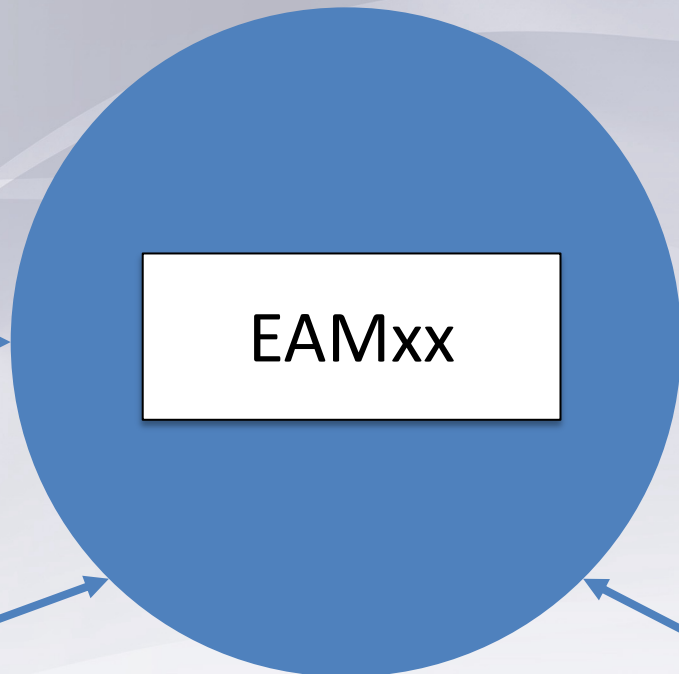


Test Name	Result	Duration
proc	Passed	
atmosphere_density	Passed	2s 9m
bfhash	Passed	1s 70m
catch_main_invalid_flags	Passed	5s
catch_main_tests	Passed	3s 350ms
check_subcycling	Passed	60ms
check_subcycling_tend_check	Passed	
check_surf_mom_flux_slices_np1	Passed	
V_slices_fail_diff	Passed	
fail_layout	Passed	

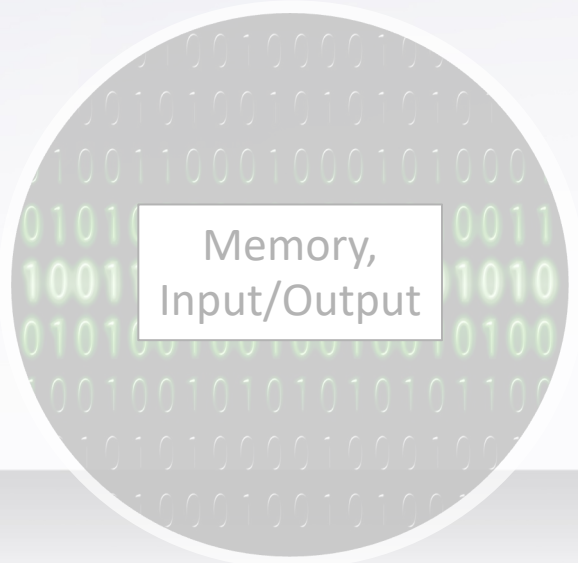
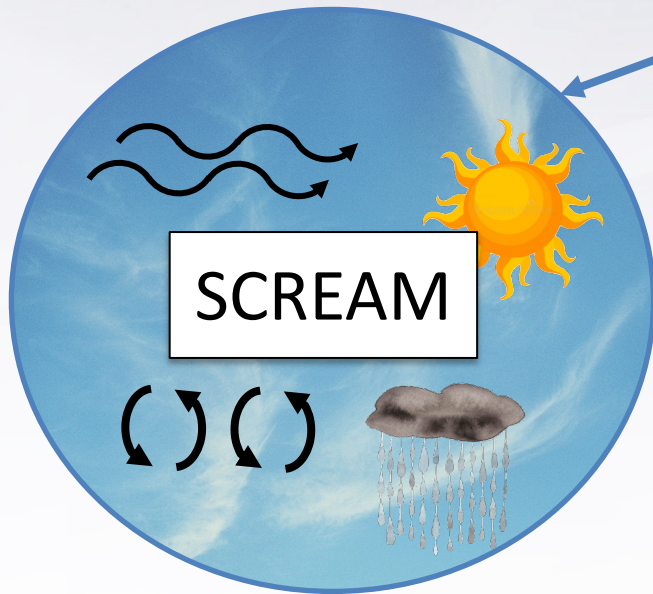


```

scmlon = 262.5
use_hetfrz_classnuc = .true.
micro_mg_dcs_tdep = .true.
microp_aero_wsub_scheme = 1
sscav_tuning = .true.
convproc_de_aer = true
demot
liqcf
regen_fix = false
resus_fix = .false.
mam_amicphys_optaa = 1
fix_g1_err_ndrop = .true.
ssalt_tuning = .true.
relvar_fix = .true.
mg_prc_coeff_fix = .true.
tmg temp fix = true
  
```


A table showing test results for various components. The word 'Testing' is written in a box in the center of the table. The table has columns for test names, status, and time taken.

Test Name	Status	Time
proc	Passed	
atmosphere_density	Passed	2s 9
bfbhash	Passed	1s 70m
catch_main_invalid_flags	Passed	5s
catch_main_tests	Passed	3s 350ms
check_subcycling	Passed	60ms
check_subcycling_tend_check	Passed	
ck_surf_mom_flux_slices_np1	Passed	
V_slices_fail_diff	Passed	
fail_layout	Passed	

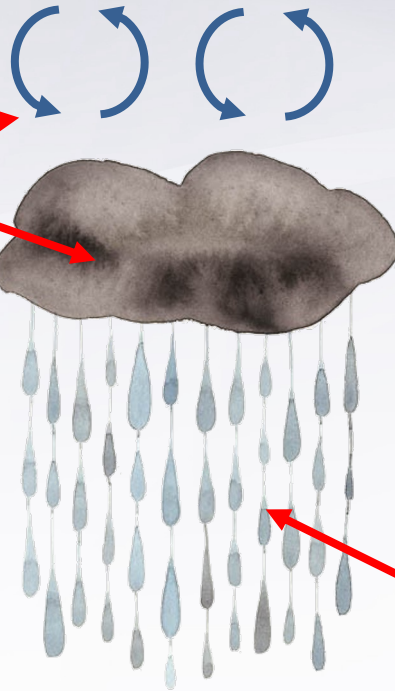
A white box containing a snippet of code for a user interface. The word 'User Interface' is written in a box in the center of the code block.

```
scmlon = 262.5
use_hetfrz_classnuc = .true.
micro_mg_dcs_tdep = .true.
microp_aero_wsub_scheme = 1
sscav_tuning = .true.
convproc_de_aer = true
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regen
resus_fix = .false.
mam_amicphys_optaa = 1
fix_g1_err_ndrop = .true.
ssalt_tuning = .true.
relvar_fix = .true.
mg_prc_coeff_fix = .true.
img temp fix = true
```

What is SCREAM? EAMxx?

- The Simple Cloud Resolving E3SM Atmosphere Model (SCREAM) is the 3.25km configuration of **EAMxx**.
- EAMxx is the atmosphere model *code* which can be run at any resolution (eventually):
 - a **complete redesign** of the E3SM Atm. Model in **C++/Kokkos**

Turbulence and cloud formation handled by Simplified Higher-Order Closure (**SHOC**)



Resolved-scale **fluid dynamics** treated by a non-hydrostatic Spectral Element (**SE**) approach



Radiation handled by externally-developed, GPU-ready **RRTMGP** package

~~parameterized convection~~

turbulent mtn. stress

Aerosols are prescribed following the Simple Prescribed Aerosols (**SPA**) model.

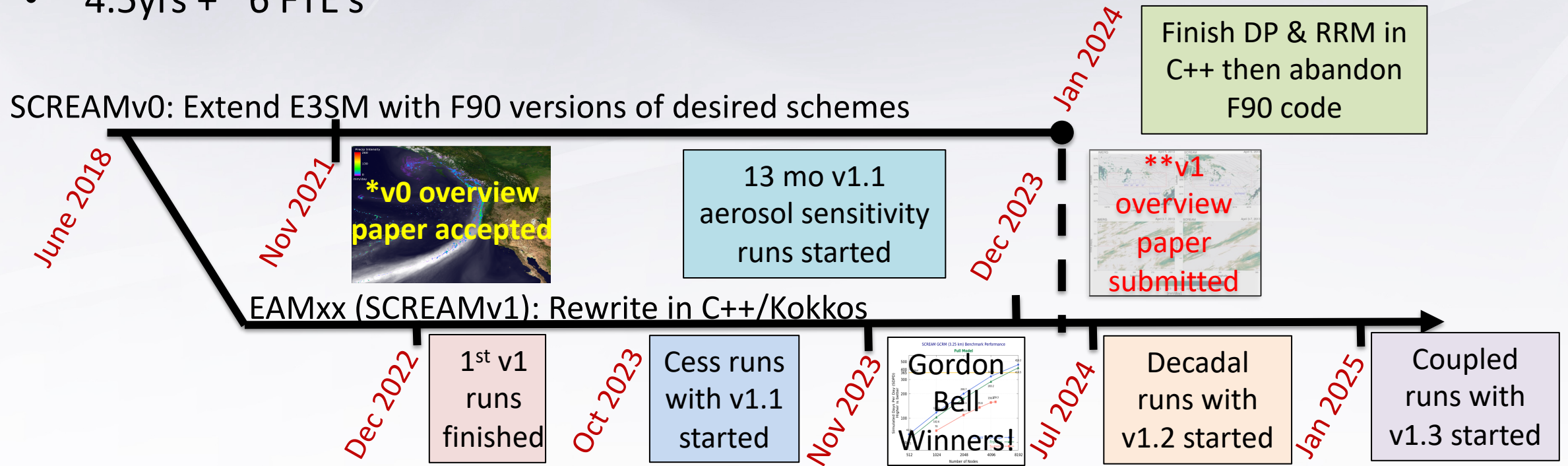
Microphysical processes handled by Predicted Particle Properties (**P3**) scheme

New to E3SM

* Using coarser grid for physics parameterizations (PG2) *

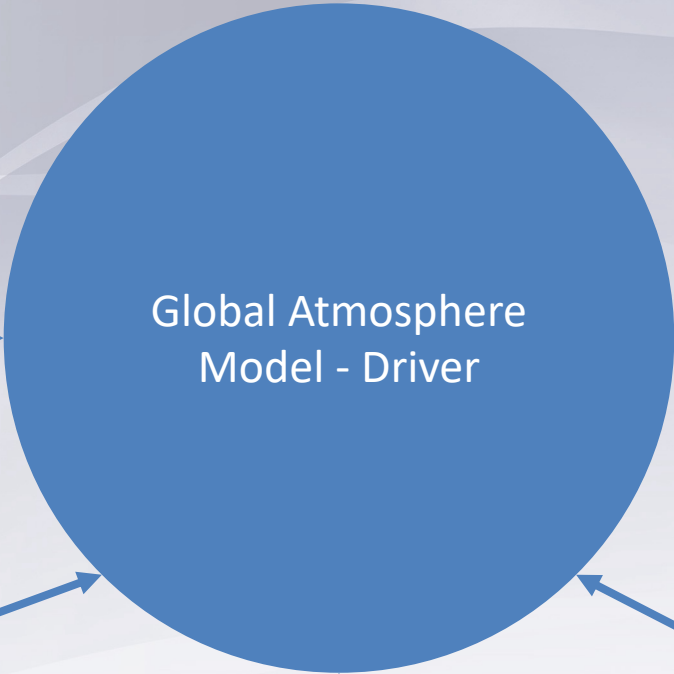
How we got here

- Parallel tracks:
 - validation of SCREAM configuration,
 - and development of EAMxx infrastructure.
- ~4.5yrs + ~6 FTE's

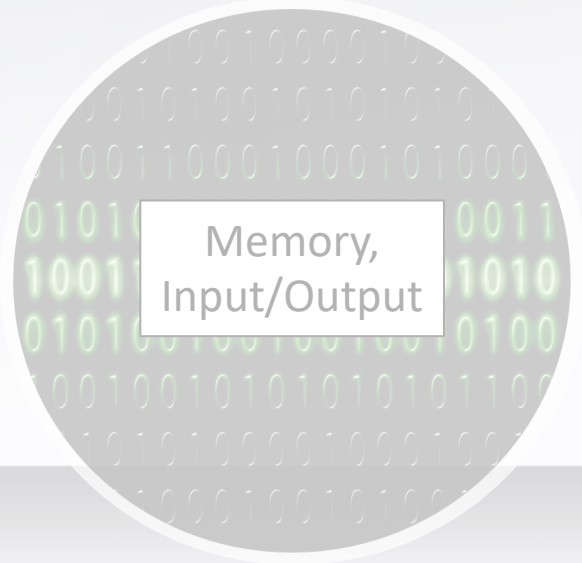
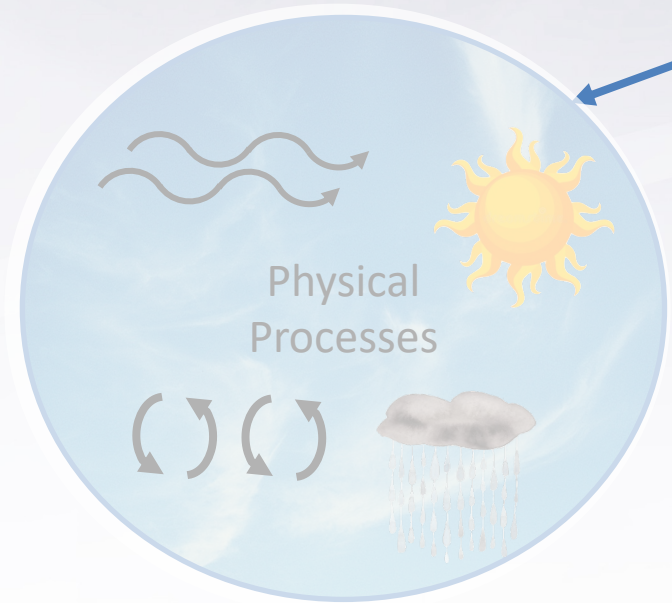


* Caldwell, PM, et al., "Convection-permitting simulations with the E3SM global atmosphere model" (2019), JAMES, doi: 0.1029/2019MS001870

** Donahue, AS, et al., "To exascale and beyond -- The Simple Cloud-Resolving E3SM Atmosphere Model (SCREAM), a performance portable global atmosphere model for cloud-resolving scales" (2024), JAMES, *under review*



Test Name	Status	Duration
proc	Passed	
atmosphere_density	Passed	2s 9m
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catch_main_invalid_flags	Passed	5s
catch_main_tests	Passed	3s 350ms
check_subcycling	Passed	60ms
check_subcycling_tend_check	Passed	
check_surf_mom_flux_slices_np1	Passed	
V_slices_fail_diff	Passed	
fail_layout	Passed	



```

scmlon = 262.5
use_hetfrz_classnuc = .true.
micro_mg_dcs_tdep = .true.
microp_aero_wsub_scheme = 1
sscav_tuning = .true.
convproc_de_aer = true
demot
liqcf
regen
resus_fix = .false.
mam_amicphys_optaa = 1
fix_g1_err_ndrop = .true.
ssalt_tuning = .true.
relvar_fix = .true.
mg_prc_coeff_fix = .true.
tmp temp fix = true
  
```


Portability and Performance

- Portable Performance:
 - Compiler Directives, e.g. OpenMP, OpenACC
 - General Purpose Libraries, e.g. Kokkos, YAKL and Raja
 - Domain Specific Languages (DSL), e.g. GridTools, PSyclone and CLAW
- Transition to C++
 - Necessary to leverage tools like Kokkos
 - Attracts the next generation of software engineers, who may have never worked with Fortran
 - Better compiler support from vendors
 - A number of added benefits, such as object oriented programming.

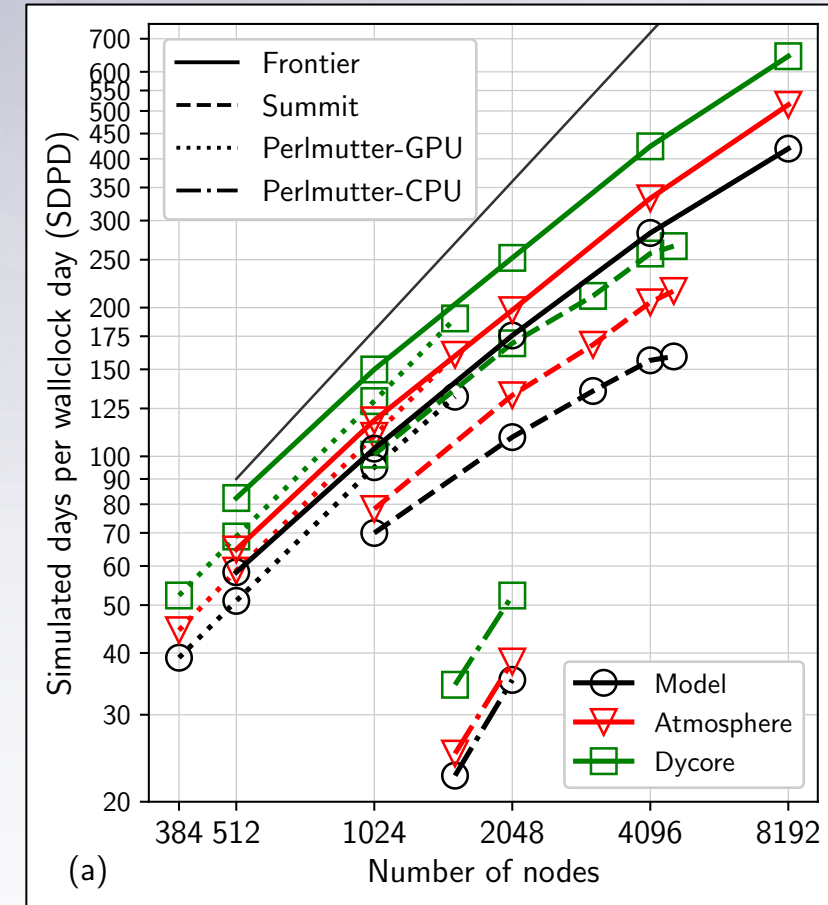
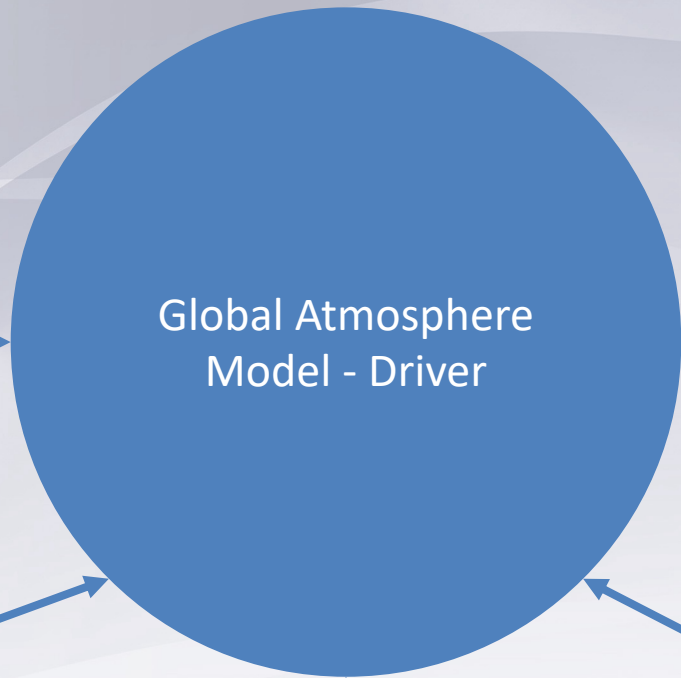
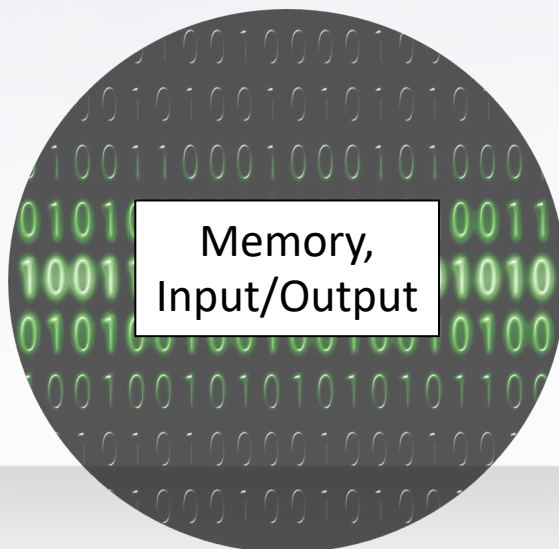
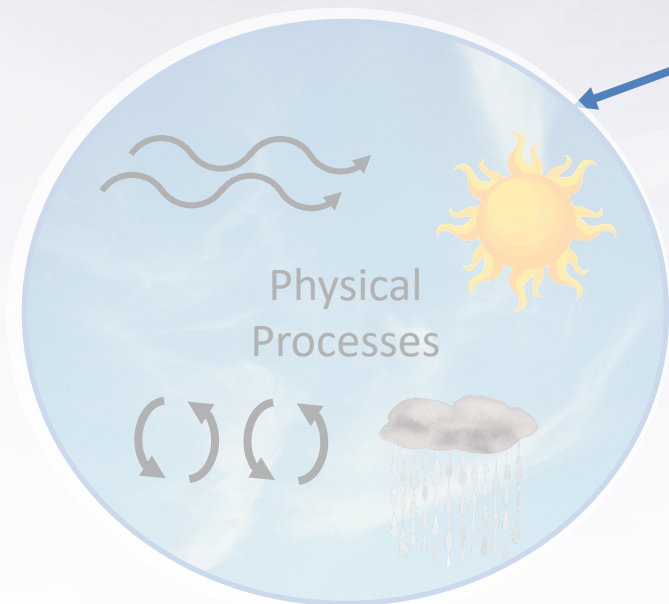


figure: scaling performance of EAMxx

Added Bonus: A complete rewrite allows us to cleanup legacy code that is either unused or rigid!



Test Name	Status	Duration
proc	Passed	
atmosphere_density	Passed	2s 9m
bfbbash	Passed	1s 70m
catch_main_invalid_flags	Passed	5s
catch_main_tests	Passed	3s 350ms
check_subcycling	Passed	60ms
check_subcycling_tend_check	Passed	
check_surf_mom_flux_slices_np1	Passed	
V_slices_fail_diff	Passed	
fail_layout	Passed	



```

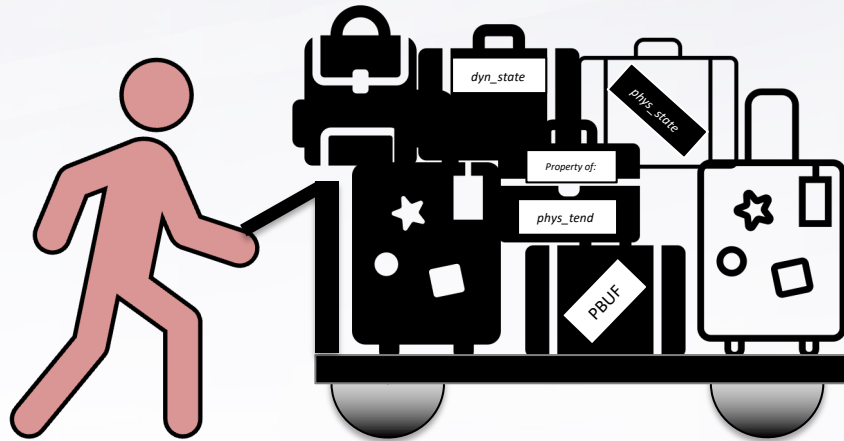
scmlon = 262.5
use_hetfrz_classnuc = .true.
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fix_g1_err_ndrop = .true.
ssalt_tuning = .true.
relvar_fix = .true.
mg_prc_coeff_fix = .true.
tmp temp fix = true
  
```


Memory Management

- 3.25km \rightarrow 25.17M columns... x 128 levels = 3.22B dofs
- Output:
 - 2D field (e.g. surface pressure) = 12.9 GB
 - 3D physics field (e.g. temperature) = 1.65 TB
 - 4x greater on dynamics grid (e.g. for restarts)

Rigid Structure

- Hard-coded persistent variables
(*phys_state*, *phys_tend*, *dyn_state*, *PBUF*)
- Hard-coded set of restart variables



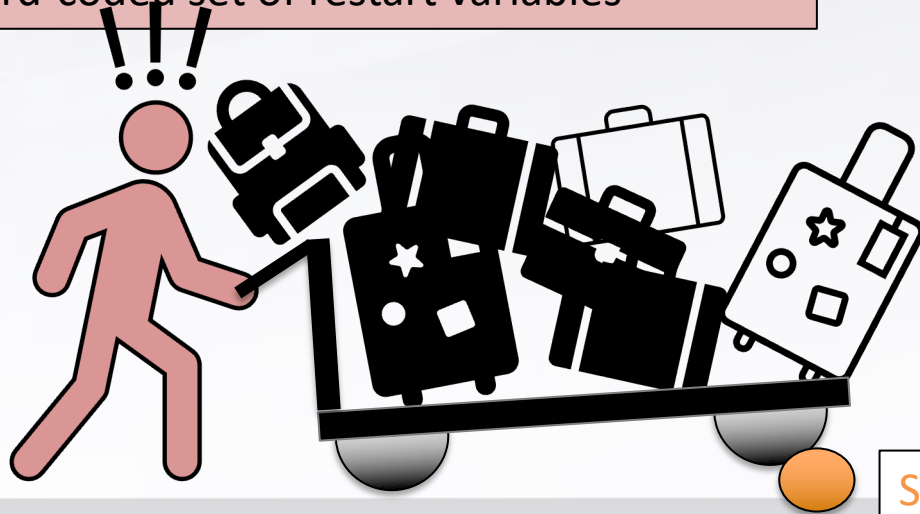
Storage & on-node memory limits

Memory Management

- 3.25km \rightarrow 25.17M columns... x 128 levels = **3.22B** dofs
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Intelligent Memory Management

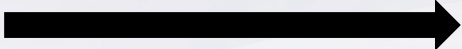
- Field Manager:
 - only allocate persistent variables actually used.
 - Restart variables list determined at runtime.
- Atm. Memory buffer – shared memory space for local variables.



Storage & on-node memory limits

The EAMxx Field Manager

phys_state
phys_tend
dyn_state
PBUF
cam_in/out



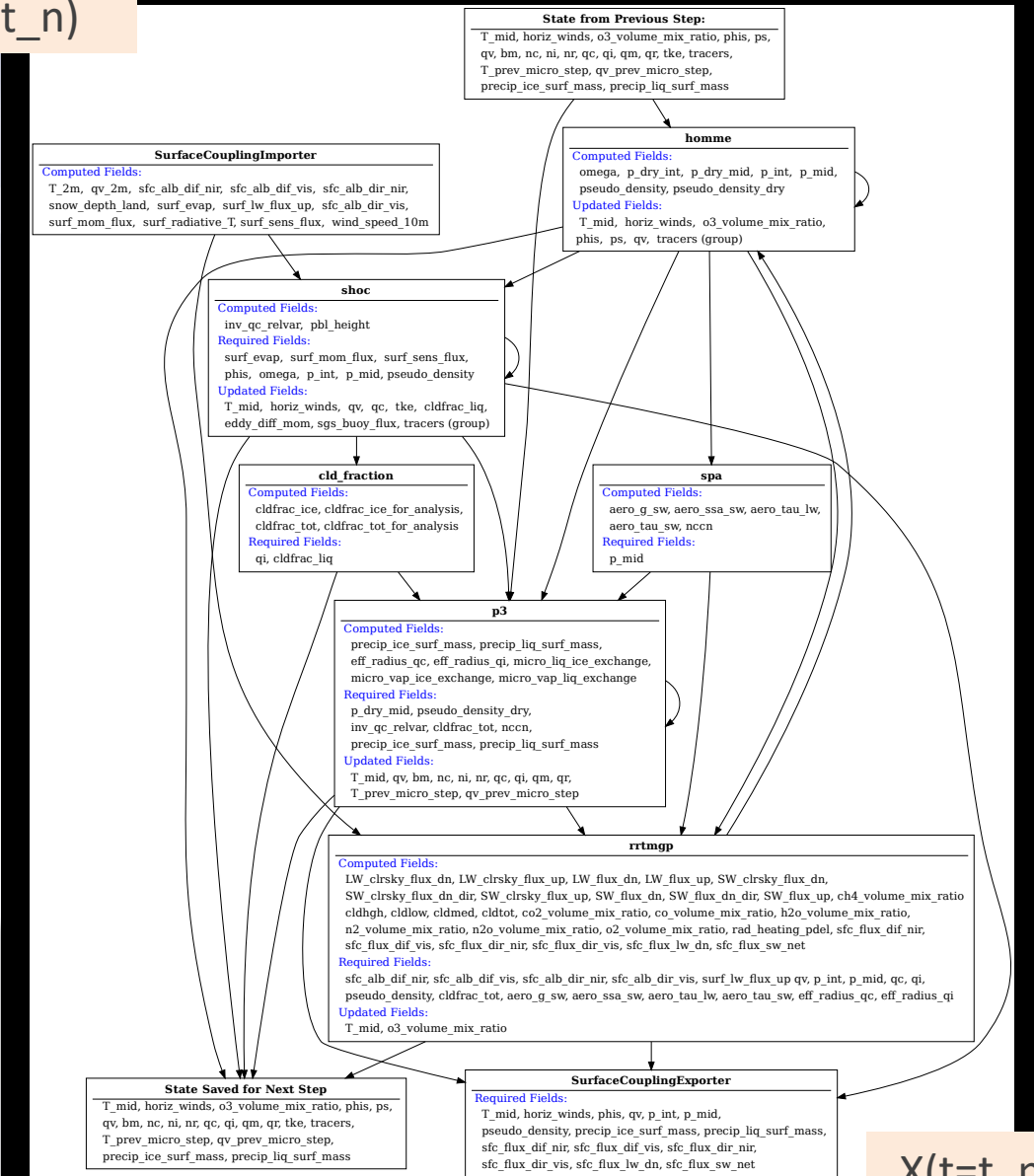
Field Manager Class and **Field Objects**

- **All persistent variables** are instances of a field object
- All fields managed by a **single Field Manager**
- Simplifies operations on fields, e.g.
 - Remapping to different grids
 - Adding new fields
 - Storing field metadata

Directed Acyclic Graph (DAG)

- Reference for **how** state variables are used.
- Quickly **audit** all global variables in the simulation.
- Runtime determination of what is needed for restarts.

$X(t=t_n)$



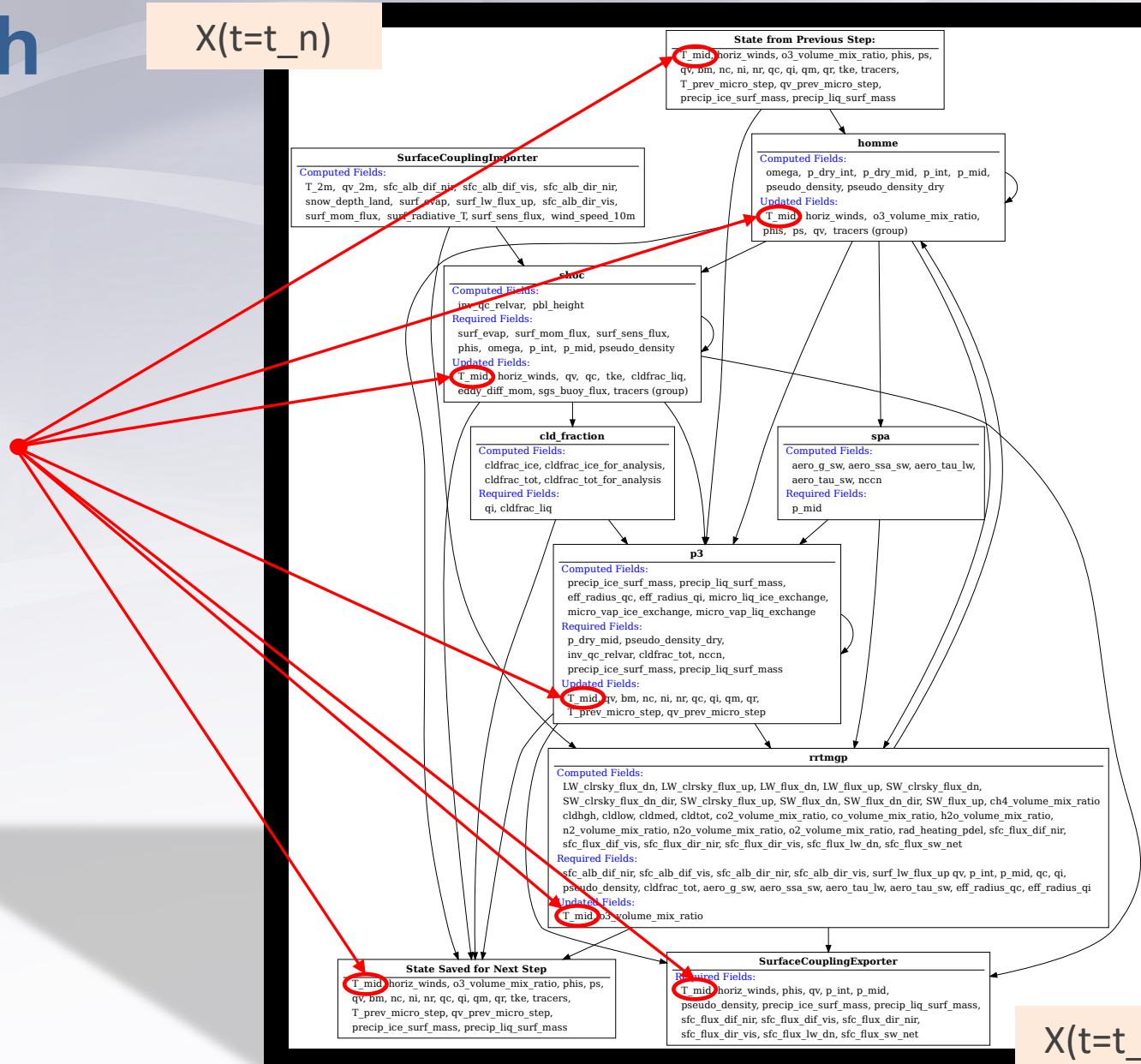
$X(t=t_{n+1})$

Directed Acyclic Graph (DAG)

- Reference for **how** state variables are used.
- Quickly **audit** all global variables in the simulation.
- Runtime determination of what is needed for restarts.

Incredibly useful for **debugging!**

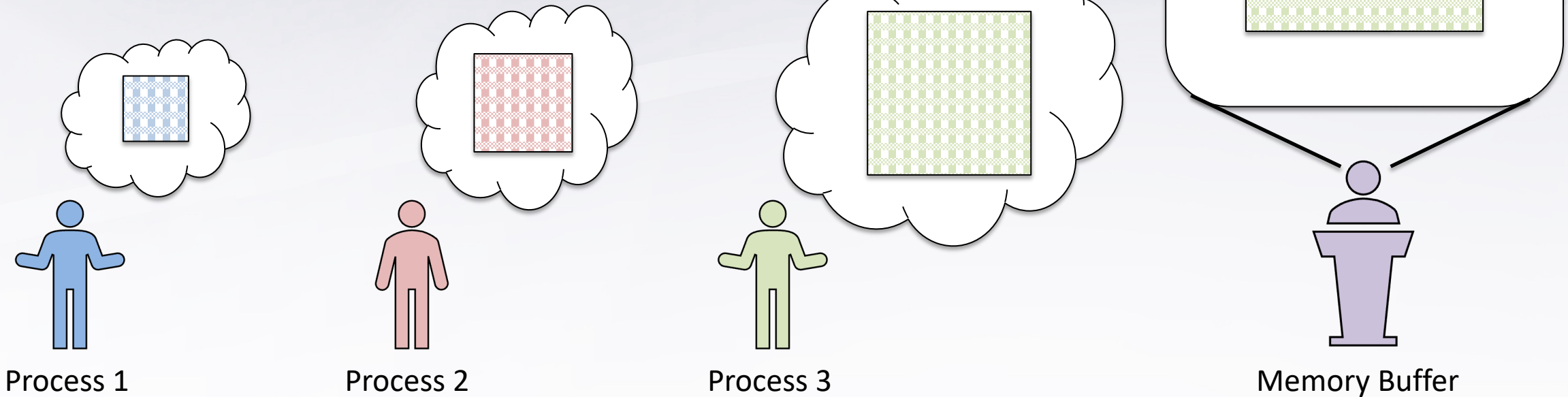
$X(t=t_n)$



$X(t=t_{n+1})$

Atmosphere memory buffer

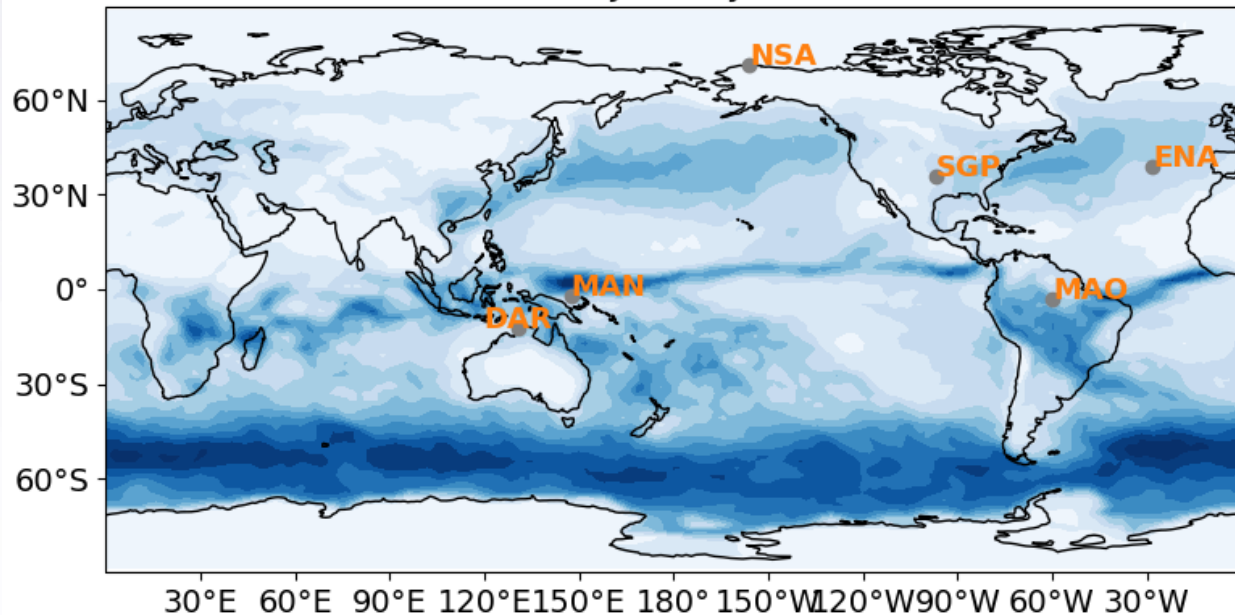
- Allocate the **minimum** memory footprint to accommodate local memory needs of all processes.
- Take advantage of pointers to memory, rather than allocated arrays.



Managing output

- 2D field (e.g. surface pressure) = 12.9 GB
- 3D physics field (e.g. temperature) = 1.65 TB
- 4x greater on dynamics grid (e.g. for restarts)

Top of Atmosphere Shortwave Cloud Forcing in SCREAMv1
January

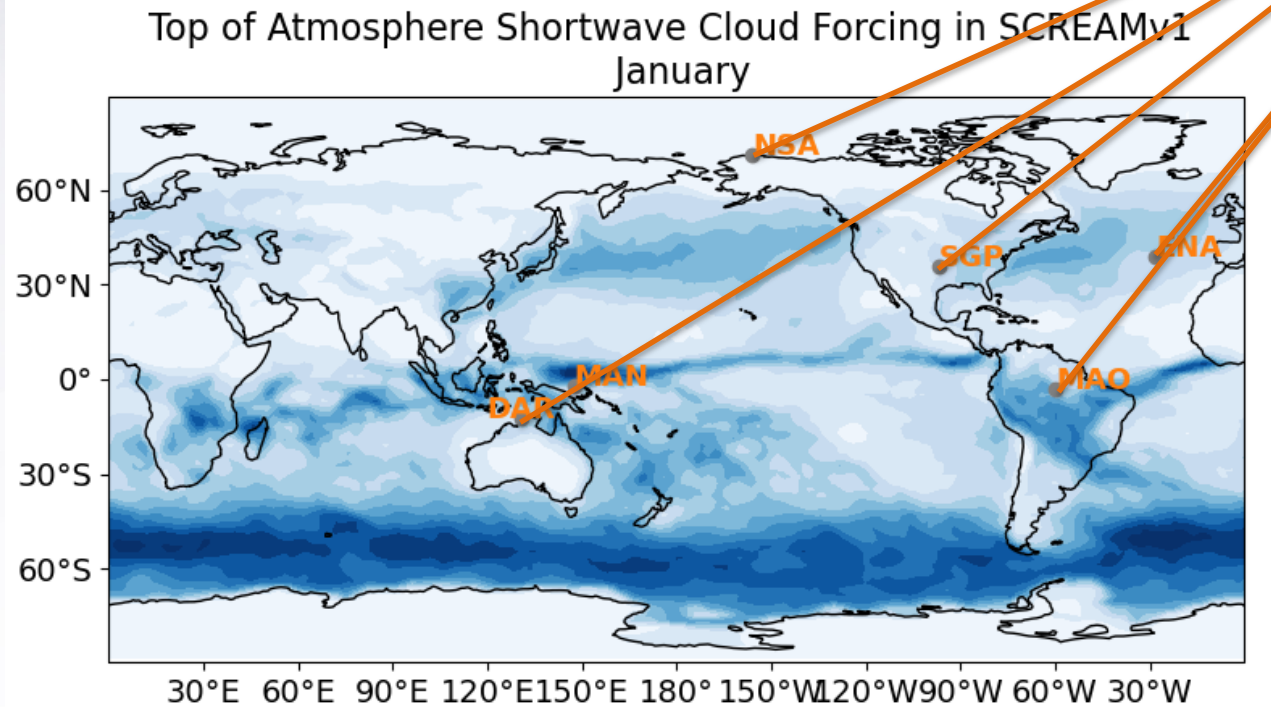


Managing output

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- 4x greater on dynamics grid (e.g. for restarts)

- NSA
- SGP
- ENA,...

Produce output at a set of distinct points.



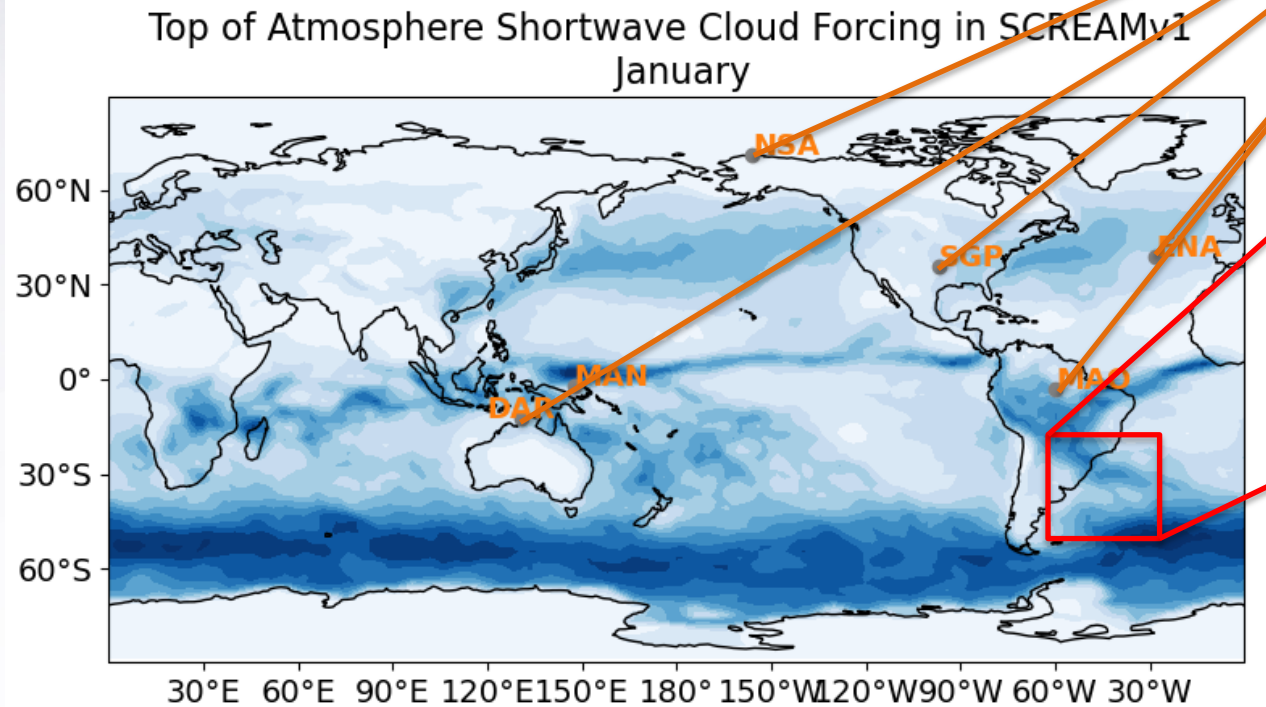
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- 2D field (e.g. surface pressure) = 12.9 GB
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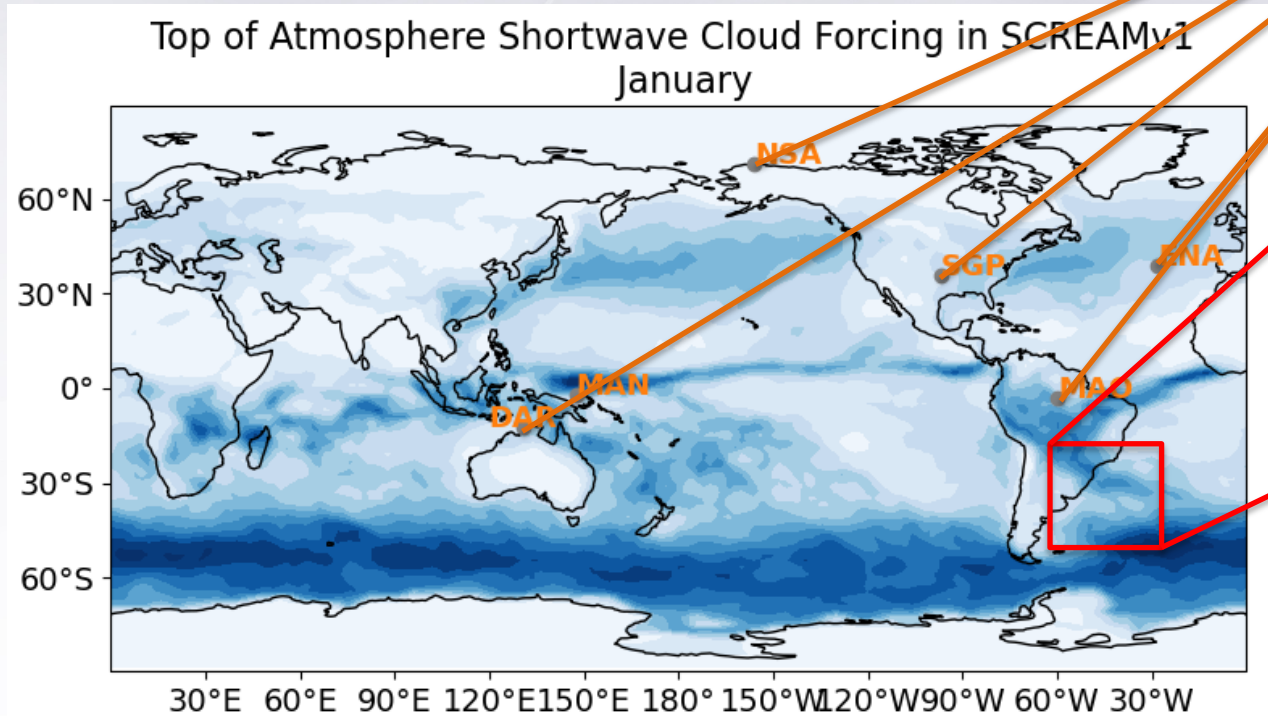
Produce output at a set of distinct points.

Produce output over a sub-region of the globe.



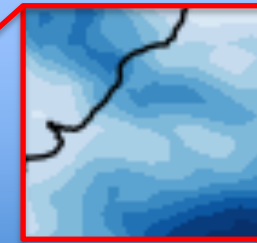
Managing output

- 2D field (e.g. surface pressure) = 12.9 GB
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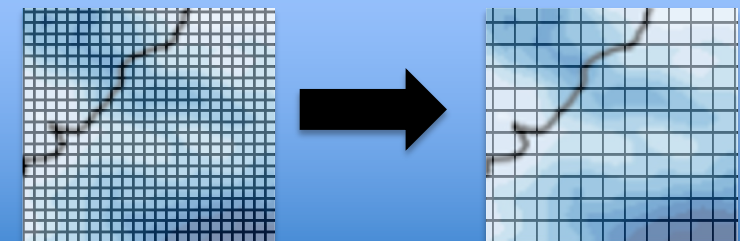
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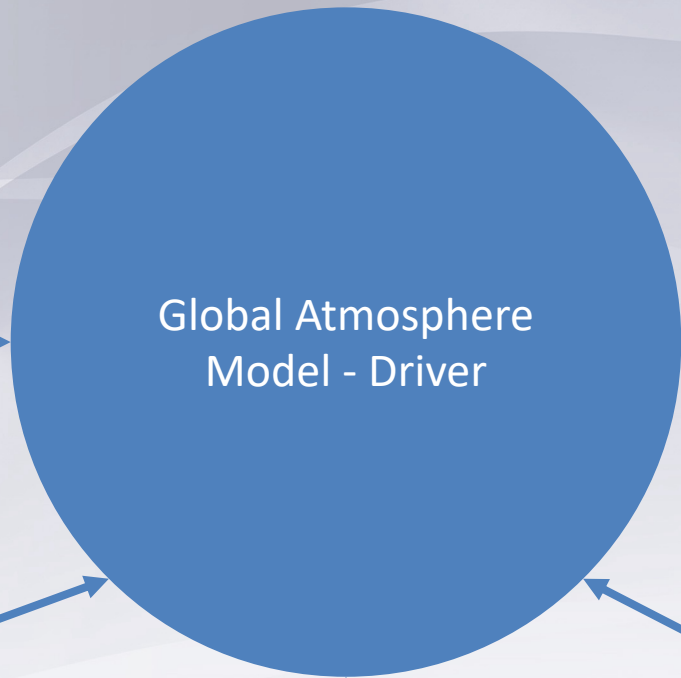
Produce output at a set of distinct points.



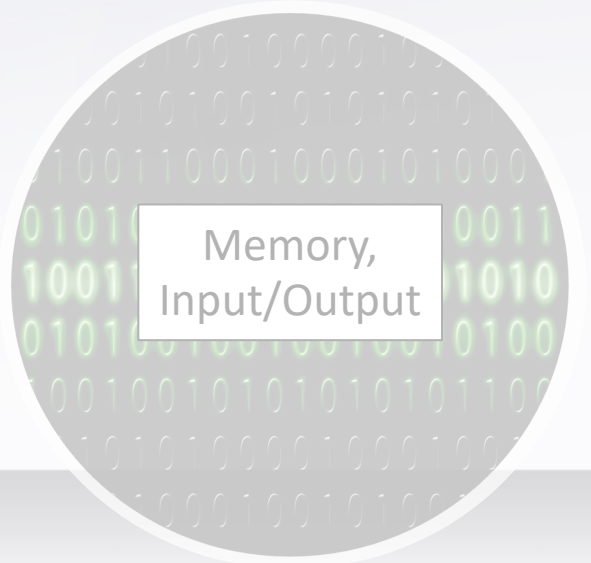
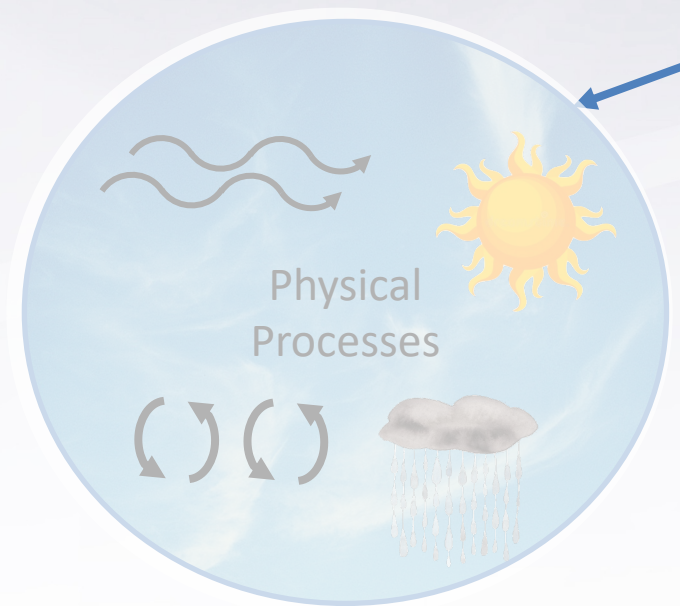
Produce output over a sub-region of the globe.

Online coarsening of output.





Test Name	Status	Duration
proc	Passed	
atmosphere_density	Passed	2s 9m
bfhash	Passed	1s 70m
catch_main_invalid_flags	Passed	5s
catch_main_tests	Passed	3s 350ms
check_subcycling	Passed	60ms
check_subcycling_tend_check	Passed	
check_surf_mom_flux_slices_np1	Passed	
V_slices_fail_diff	Passed	
fail_layout	Passed	

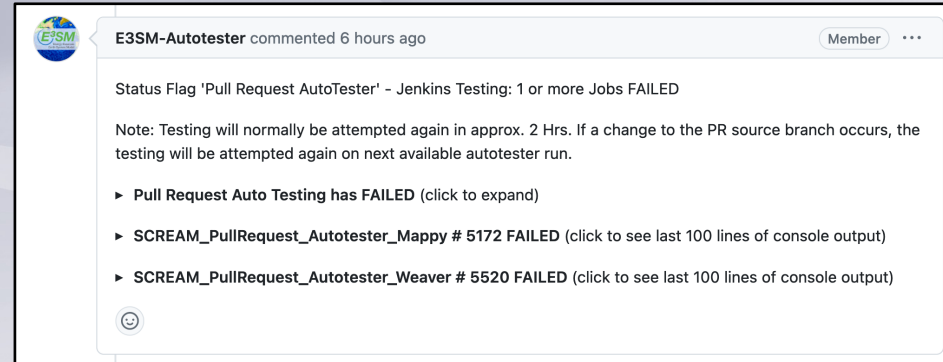


```

scmlon = 262.5
use_hetfrz_classnuc = .true.
micro_mg_dcs_tdep = .true.
microp_aero_wsub_scheme = 1
sscav_tuning = .true.
convproc_de_aer = true
demot
liqcf
regen
resus_fix = .false.
mam_amicphys_optaa = 1
fix_g1_err_ndrop = .true.
ssalt_tuning = .true.
relvar_fix = .true.
mg_prc_coeff_fix = .true.
img temp fix = true
  
```

Testing

- EAMxx inherits all the standard E3SM testing coverage, + **robust unit tests**
- This is possible because,
 - Model elements are **independent**.
 - Take advantage of arbitrary class structure in C++.
- Incredibly useful for **debugging** and **verification**
- SCREAM git-repo CI integrates unit testing through the Autotester.



E3SM-Autotester commented 6 hours ago

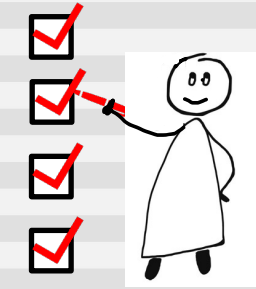
Status Flag 'Pull Request AutoTester' - Jenkins Testing: 1 or more Jobs FAILED

Note: Testing will normally be attempted again in approx. 2 Hrs. If a change to the PR source branch occurs, the testing will be attempted again on next available autotester run.

- ▶ Pull Request Auto Testing has FAILED (click to expand)
- ▶ SCREAM_PullRequest_Autotester_Mappy # 5172 FAILED (click to see last 100 lines of console output)
- ▶ SCREAM_PullRequest_Autotester_Weaver # 5520 FAILED (click to see last 100 lines of console output)

477 tests passed.

Name ^	Status ^	Time	History	Summary
ad_ut	Passed	2s 140ms	Stable	Stable
array_io	Passed	3s 230ms	Stable	Stable
atm_proc	Passed	2s 680ms	Stable	Stable
atmosphere_density	Passed	1s 460ms	Stable	Stable
bfbhash	Passed	3s 730ms	Stable	Stable
catch_main_invalid_flags	Passed	3s 990ms	Stable	Stable
catch_main_tests	Passed	3s 640ms	Stable	Stable
check_subcycling	Passed	50ms	Stable	Stable
check_subcycling_tend_check	Passed	320ms	Stable	Stable
check_surf_mom_flux_slices_np1	Passed	370ms	Stable	Stable
check_surf_mom_flux_slices_np2	Passed	380ms	Stable	Stable
check_surf_mom_flux_slices_np3	Passed	340ms	Stable	Stable
check_surf_mom_flux_slices_np4	Passed	370ms	Stable	Stable
check_U_V_slices_fail_diff	Passed	310ms	Stable	Stable
check_U_V_slices_fail_layout	Passed	390ms	Stable	Stable
check_U_V_slices_fail_missing	Passed	350ms	Stable	Stable
check_U_V_slices_np1	Passed	470ms	Stable	Stable
check_U_V_slices_np2	Passed	360ms	Stable	Stable
check_U_V_slices_np3	Passed	370ms	Stable	Stable
check_U_V_slices_np4	Passed	340ms	Stable	Stable
cid_fraction_standalone	Passed	1s 570ms	Stable	Stable
coarsening_remapper_np1	Passed	3s 400ms	Stable	Stable
coarsening_remapper_np2	Passed	2s 620ms	Stable	Stable
coarsening_remapper_np3	Passed	1s 180ms	Stable	Stable
coarsening_remapper_np4	Passed	820ms	Stable	Stable



Runtime Options:

```
cld_macmic_num_steps = 6
mfilt = 10000,1,12
cosp_lite = .true.
use_gw_front = .true.
nhtfrq = 1,0,-2
fincl1 = 'Q', 'CLDLIQ', 'CLDICE'
fincl2 = 'PS', 'TMQ', 'T500'
scm_iop_srf_prop = .true.
avgflag_pertape = 'A'
iop_nudge_tq = .false.
cld_macmic_num_steps
iradlw = 1
iradsw = 1
iopfile = '/usr/gdata
precip_off = .false.
scmlat = 36.6
scmlon = 262.5
use_hetfrz_classnuc =
micro_mg_dcs_tdep = .
microp_aero_wsub_sche
sscav_tuning = .true.
convproc_do_aer = .tr
demott_ice_nuc = .tru
liqcf_fix = .true.
regen_fix = .true.
resus_fix = .false.
mam_amicphys_optaa =
fix_g1_err_ndrop = .t
ssalt_tuning = .true.
relvar_fix = .true.
mg_prc_coeff_fix = .true.
rrtmg_temp_fix = .true.
mam_amicphys_optaa = 1
fix_g1_err_ndrop = .true.
ssalt_tuning = .true.
use_rad_dt_cosz = .true.
ice_sed_ai = 500.0
do_tms = .false.
n_so4_monolayers_pcase = 8.0D0
se_ftype = 2
zmconv_trigdcape_ull = .true.
cld_sed = 1.0D0
effgw_beres = 0.35
gw_convect_hcf = 12.5
effaw_oro = 0.375
```

cld_macmic_num_steps = 6

```
mfilt = 10000,1,12
cosp_lite = .true.
use_gw_front = .true.
nhtfrq = 1,0,-2
fincl1 = 'Q', 'CLDLIQ', 'CLDICE'
fincl2 = 'PS', 'TMQ', 'T500'
scm_iop_srf_prop = .true.
avgflag_pertape = 'A', 'I', 'X'
iop_nudge_tq = .false.
```

cld_macmic_num_steps = 3

- Difficult to read/parse
- Not organized
- Cumbersome to add new options
- Difficult to audit, vulnerable to user error
 - Conflicts only detected if developer adds their own checks.
 - Multiple entries can lead to unexpected behavior.

Runtime Options: YAML

- EAMxx use YAML to handle all runtime options.
- **Human readable** – options organized into relevant sections.
- Strict enforcement of each entry.
- Support for “info” metadata for user support.
- Setting and adding new options is simple. **Each process has their own parameter list.**
- Has **similar support to CIME XML** functions
 - `./atmchange`
 - `./atmquery`

```
physics:
  Type: Group
  atm_procs_list: !strings
  - mac_aero_mic
  - rrtmgp
  - mlcorrection
  compute_tendencies: !strings
  - T_mid
  - qv
  - horiz_winds
  enable_postcondition_checks: true
  enable_precondition_checks: true
  internal_diagnostics_level: 0
  mac_aero_mic:
    Type: Group
    atm_procs_list: !strings
    - tms
    - shoc
    - cldFraction
    - spa
    - p3
    cldFraction:
      compute_tendencies: !strings []
      enable_postcondition_checks: true
      enable_precondition_checks: true
      internal_diagnostics_level: 0
      number_of_subcycles: 1
      repair_log_level: trace
    compute_tendencies: !strings []
    enable_postcondition_checks: true
    enable_precondition_checks: true
    internal_diagnostics_level: 0
    number_of_subcycles: 12
  p3:
    compute_tendencies: !strings []
    do_predict_nc: true
    do_prescribed_ccn: true
    enable_column_conservation_checks: false
    enable_postcondition_checks: true
    enable_precondition_checks: true
    internal_diagnostics_level: 0
    max_total_ni: 740000.0
    number_of_subcycles: 1
    p3_a_imm: 0.65
    p3_autoconversion_prefactor: 1350.0
```

Runtime Options: YAML

```
> ./atmquery mac_aero_mic::number_of_subcycles
namelist_defaults::atmosphere_processes::physics::mac_aero_mic::number_of_subcycles: 6
> ./atmchange mac_aero_mic::number_of_subcycles=12
Regenerating .../namelist_scream.xml. Manual edits will be lost.
> ./atmquery mac_aero_mic::number_of_subcycles
namelist_defaults::atmosphere_processes::physics::mac_aero_mic::number_of_subcycles: 12
```

- EAMxx

- Human

- Strict e

- Support

- Setting

their c

- Has sim

- ./

- ./

```
mac_aero_mic:
  Type: Group
  atm_procs_list: !strings
  - tms
  - shoc
  - cldFraction
  - spa
  - p3
  cldFraction:
    compute_tendencies: !strings []
    enable_postcondition_checks: true
    enable_precondition_checks: true
    internal_diagnostics_level: 0
    number_of_subcycles: 1
    repair_log_level: trace
  compute_tendencies: !strings []
  enable_postcondition_checks: true
  enable_precondition_checks: true
  internal_diagnostics_level: 0
  number_of_subcycles: 12
```

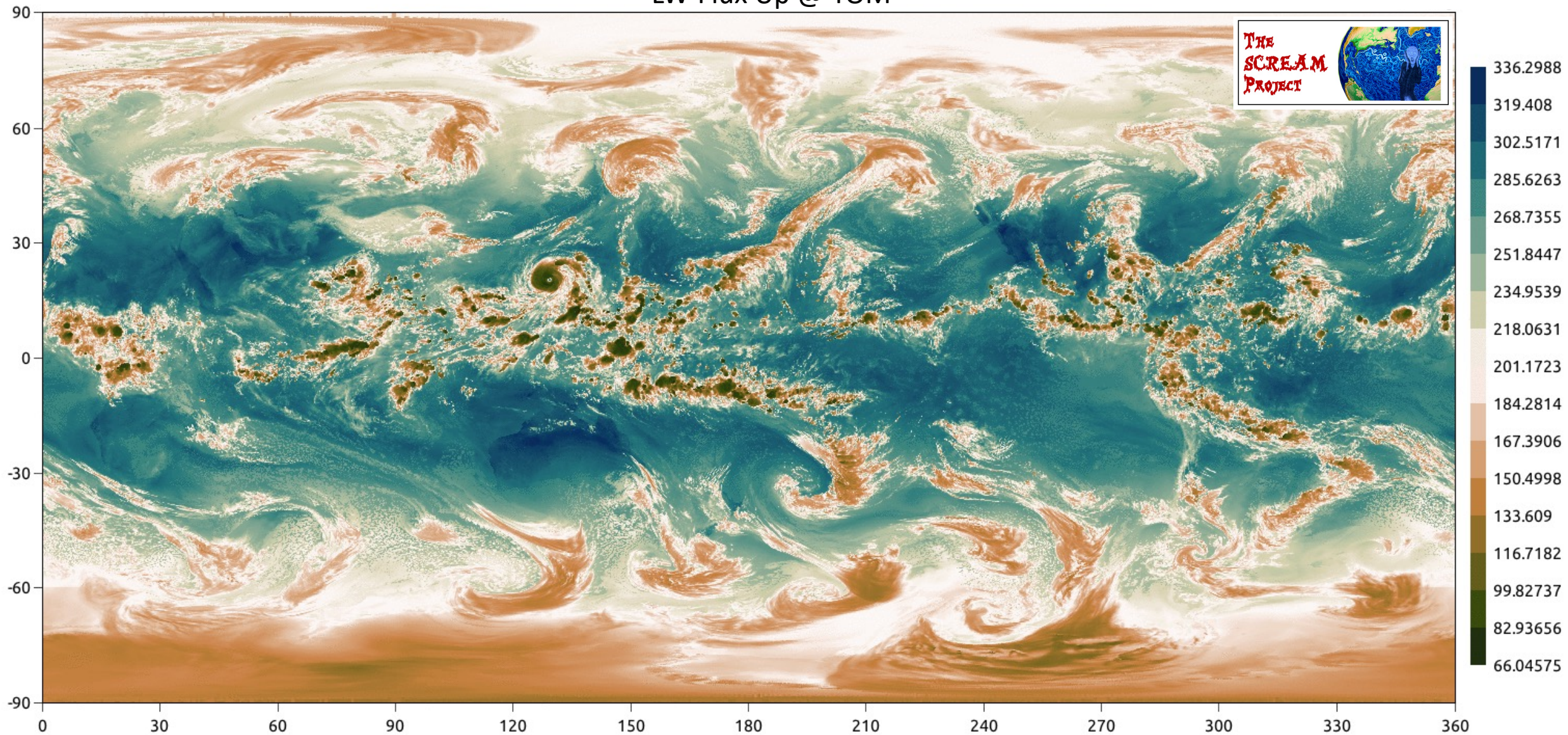
ections.

cess has

```
- horiz_winds
enable_postcondition_checks: true
enable_precondition_checks: true
internal_diagnostics_level: 0
mac_aero_mic:
  Type: Group
  atm_procs_list: !strings
  - tms
  - shoc
  - cldFraction
  - spa
  - p3
  cldFraction:
    compute_tendencies: !strings []
    enable_postcondition_checks: true
    enable_precondition_checks: true
    internal_diagnostics_level: 0
    number_of_subcycles: 1
    repair_log_level: trace
  compute_tendencies: !strings []
  enable_postcondition_checks: true
  enable_precondition_checks: true
  internal_diagnostics_level: 0
  number_of_subcycles: 12
p3:
  compute_tendencies: !strings []
  do_predict_nc: true
  do_prescribed_ccn: true
  enable_column_conservation_checks: false
  enable_postcondition_checks: true
  enable_precondition_checks: true
  internal_diagnostics_level: 0
  max_total_ni: 740000.0
  number_of_subcycles: 1
  p3_a_imm: 0.65
  p3_autoconversion_prefactor: 1350.0
```


Questions? donahue5@llnl.gov

LW-Flux Up @ TOM



Output Control: user_nl_eam

```
cld_macmic_num_steps = 6
mfilt = 10000,1,12
cosp_lite = .true.
use_gw_front = .true.
nhtfrq = 1,0,-2
fincl1 = 'Q','CLDLIQ','CLDICE'
fincl2 = 'PS','TMQ','T500'
scm_iop_srf_prop = .true.
avgflag_pertape = 'A','I','X'
iop_nudge_to = false
```


Output Control: YAML

```
cld_macmic_num_steps = 6
mfilt = 10000,1,12
cosp_lite = .true.
use_gw_front = .true.
nhtfrq = 1,0,-2
fincl1 = 'Q','CLDLIQ','CLDICE'
fincl2 = 'PS','TMQ','T500'
scm_iop_srf_prop = .true.
avgflag_pertape = 'A','I','X'
iop_nudge_to = false
```

```
Scorio:
  model_restart:
    filename_prefix: ./F2010-SCREAMv1.ne30pg2_ne30pg2
    output_control:
      Frequency: 1
      frequency_units: nmonths
    output_yaml_files: !strings
  - data/my_first_output_file.yaml
  - data/my_other_output_file.yaml
```

Output Control: YAML

```
cld_macmic_num_steps = 6
mfilt = 10000,1,12
cosp_lite = .true.
use_gw_front = .true.
nhtfrq = 1,0,-2
fincl1 = 'Q','CLDLIQ','CLDICE'
fincl2 = 'PS','TMQ','T500'
scm_iop_srf_prop = .true.
avgflag_pertape = 'A','I','X'
iop_nudge_to = false
```

```
Averaging Type: Instant
Fields:
  Physics PG2:
    Field Names:
      - qv
      - qc
      - qi
Max Snapshots Per File: 1
filename_prefix: output.scream.monthly.NAME_1
output_control:
  Frequency: 1
  frequency_units: nmonths
```

```
Averaging Type: Max
Fields:
  Physics PG2:
    Field Names:
      - ps
      - VapWaterPath
      - LiqWaterPath
Max Snapshots Per File: 12
filename_prefix: output.scream.monthly.NAME_2
output_control:
  Frequency: 2
  frequency_units: nhours
```

What is a Field?

- Stores everything the atmosphere model needs to know about a global variable.
- As an object allows SCREAM to define universal operations for all fields,
 - E.g. remapping, arithmetic operations, cloning, property checking, timestep management ...

```
> Name: T_mid
> Units: K
> Layout: (columns, levels)
> Grid: Physics PG2
> Datatype: Real
> Timestamp: TS{2024,11,4,8,30,0}
> Data Pointer: 6efgkh38sahdlgis0372
> Providers: HOMME, SHOC, P3, RRTMGP, Surface-Coupling
> Customers: HOMME, SHOC, P3, RRTMGP, Surface-Coupling
> Extra Metadata: [Mask, Foo, Bar, ...]
```

* Artist depiction

What is an Atmosphere Process?

- An interface to the dynamics or an atmosphere parameterization.
- EAMxx supports universal operations on atmosphere processes:
 - Unit testing, subcycling, backing out tendencies, log msgs, performance timing, ...
- Has a defined initialization, run and finalization.

```
> Name: SHOC
> Type: Physics
> Grid: Physics PG2
> Timestamp: TS{2024,11,4,8,30,0}
> Inputs: omega, surf_sens_flux, surf_mom_flux, ..., T_mid, qv
> Outputs: surf_evap, T_mid, qv, ... , tke, pbl_height
> init_impl: Do 'xyz' to initialize SHOC
> run_impl: Do 'ijk,' then call shoc_main, do 'qrs'
> finalize_impl: Nothing to do
```

Performance Portability (C++/Kokkos)

U.S. DEPARTMENT OF ENERGY | Office of Science
Sandia National Laboratories | E³SM Energy Exascale Earth System Model | SC23 Denver, CO | am hpc.

The Simple Cloud-Resolving E3SM Atmosphere Model Running on the Frontier Exascale System

Luca Bertagna (lbtag@sandia.gov)
Sandia National Laboratories
Nov. 15th 2023

Mark Taylor, Peter Caldwell, Luca Bertagna, Conrad Clevenger, Aaron Donahue, James Foucar, Oksana Guba, Benjamin Hillman, Noel Keen, Jayesh Krishna, Matthew Norman, Sarat Sreepathi, Christopher Terai, James White, Danqing Wu, Andrew Salinger, Renata McCoy, L. Ruby Leung, David Bader

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<https://acme-climate.atlassian.net/wiki/spaces/ECM/pages/4129325057/2024-02-15+All-Hands+Presentation+Meeting+Notes>

Packs

