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MARCH 5, 2026

# Developing language interoperable atmospheric modeling software: an approach for integrating CAM Fortran parameterizations into E3SM C++ code

**Ren Stengel, John Dennis, Jian Sun, Michael Waxmonsky**

**Supported through the Community Software Facility (CSF)**

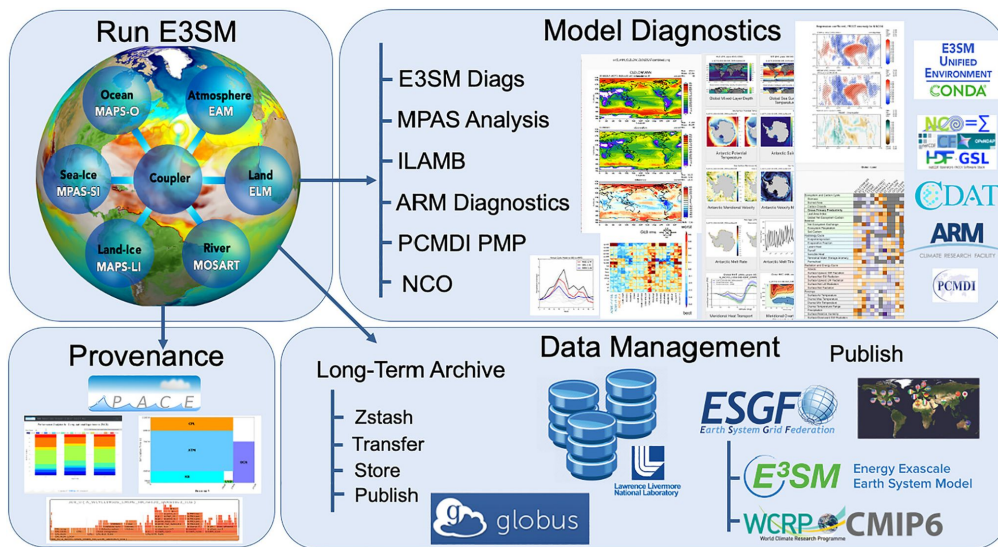
*This material is based upon work supported by the NSF National Center for Atmospheric Research, a major facility sponsored by the U.S. National Science Foundation and managed by the University Corporation for Atmospheric Research. Any opinions, findings and conclusions or recommendations expressed in this material do not necessarily reflect the views of NSF.*



- Multiple ongoing/past projects that involve code modernization
  - CCPP: Interoperable physics written in Fortran
  - Earthworks: GPU-enablement through OpenACC directives
  - StormSPEED: Integration of performance-portable Kokkos/C++ dynamical core
  - Experimentation with JAX
- Code modernization efforts have different goals
  - Complexity containment
  - Physics package portability
  - GPU-enablement
- Observations:
  - Primary industry support is: Python and C++
  - Significantly less support for Fortran and even less for Fortran on GPUs
  - Graduate students/Postdocs (i.e. **future scientific leaders**) are using Python
- How would multi-language support impact community contribution?
  - StormSPEED: C++ dynamical core in Fortran application (CAM)
  - This project: Fortran physics in Kokkos/C++ application (EAMxx)

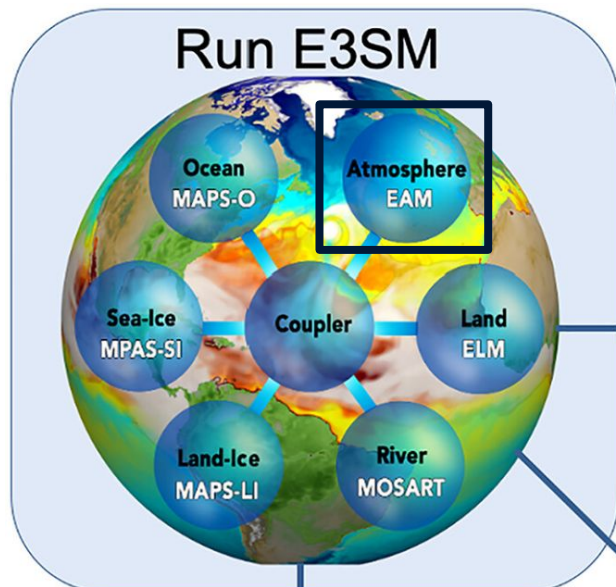
# Energy Exascale Earth System Model (E3SM)

- E3SM is DOE's earth system modeling framework
- The goal is to provide a framework capable of exascale simulations



# EAMxx – atmospheric modeling component

- **Supports language interoperability for parameterizations and physics**
- Hardware portability and performance on GPUs with Kokkos



We will focus on the atmospheric component: EAMxx

- Uses the standard `./xmlchange` functionality:
  - Select COMPSET and grid
  - Set up compilers, machine environment, and batch job parameters
  - Simulated run time, time stepping, etc

```
./xmlchange RUN_TYPE="startup"
if [[ $COMPSET == *"F20TR"* ]]; then
  ./xmlchange RUN_STARTDATE='1850-01-01'
elif [[ $COMPSET == "FMTHIST" || $COMPSET == "FLTHIST" ]]; then
  ./xmlchange RUN_STARTDATE='2001-01-01'
else
  ./xmlchange RUN_STARTDATE='0001-01-01'
fi
./xmlchange RESUBMIT='0'
./xmlchange CONTINUE_RUN='FALSE'
./xmlchange STOP_N='2',STOP_OPTION='ndays'
./xmlchange JOB_WALLCLOCK_TIME='00:15:00'
./xmlchange JOB_QUEUE=$QUEUE_NAME
./xmlchange BUDGETS=TRUE

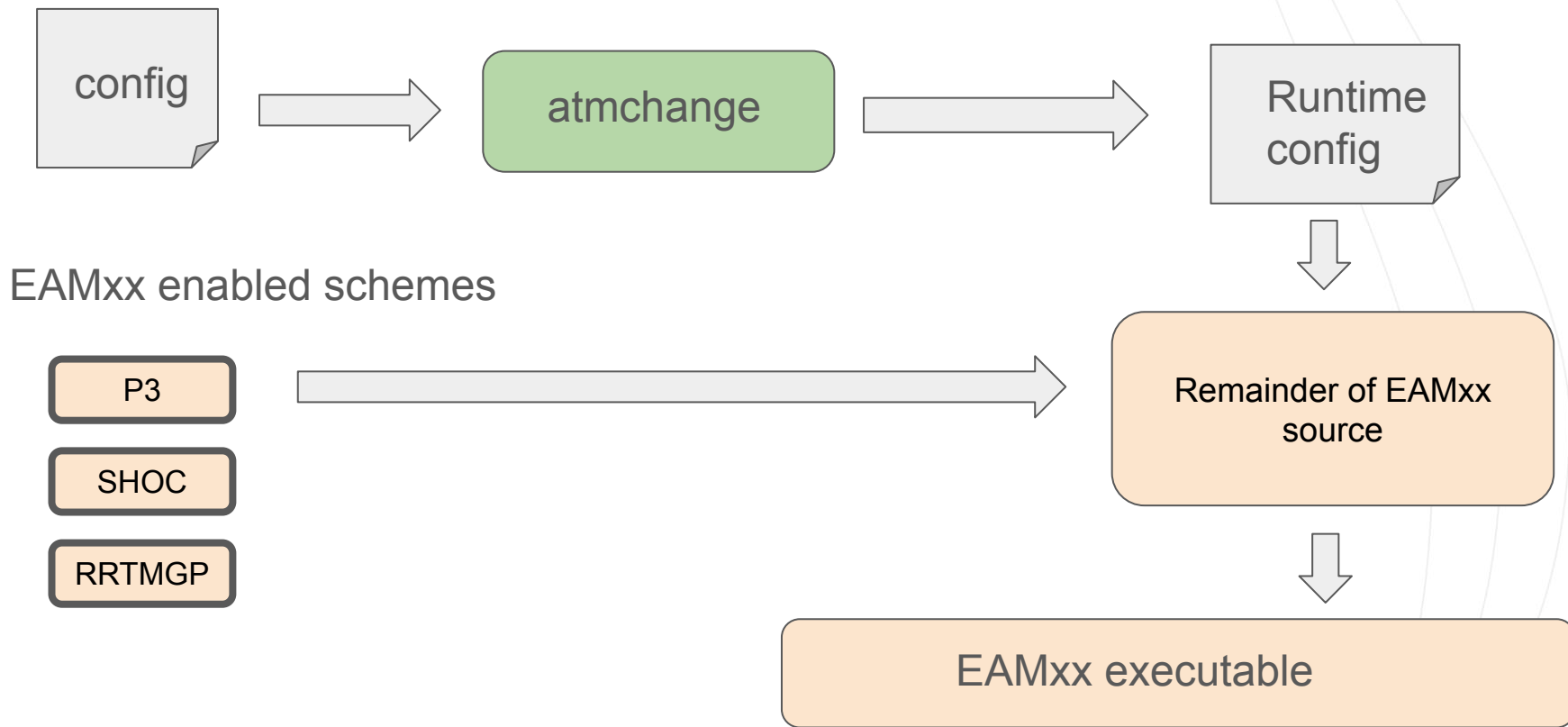
if [[ $DYCORE == "theta-l_kokkos" ]]; then
cat << EOF >> user_nl_elm
  check_finidat_year_consistency = .false.
  check_dynpft_consistency = .false.
  create_crop_landunit = .false.
EOF
fi
```

- Uses the standard `./xmlchange` functionality:
  - Select COMPSET and grid
  - Set up compilers, machine environment, and batch job parameters
  - Simulated run time, time stepping, etc
- Uses `./atmchange` to change atmospheric process settings at runtime
- CCpp (used by CAM-SIMA) uses XML files to determine atmospheric process settings which then generates code to compile

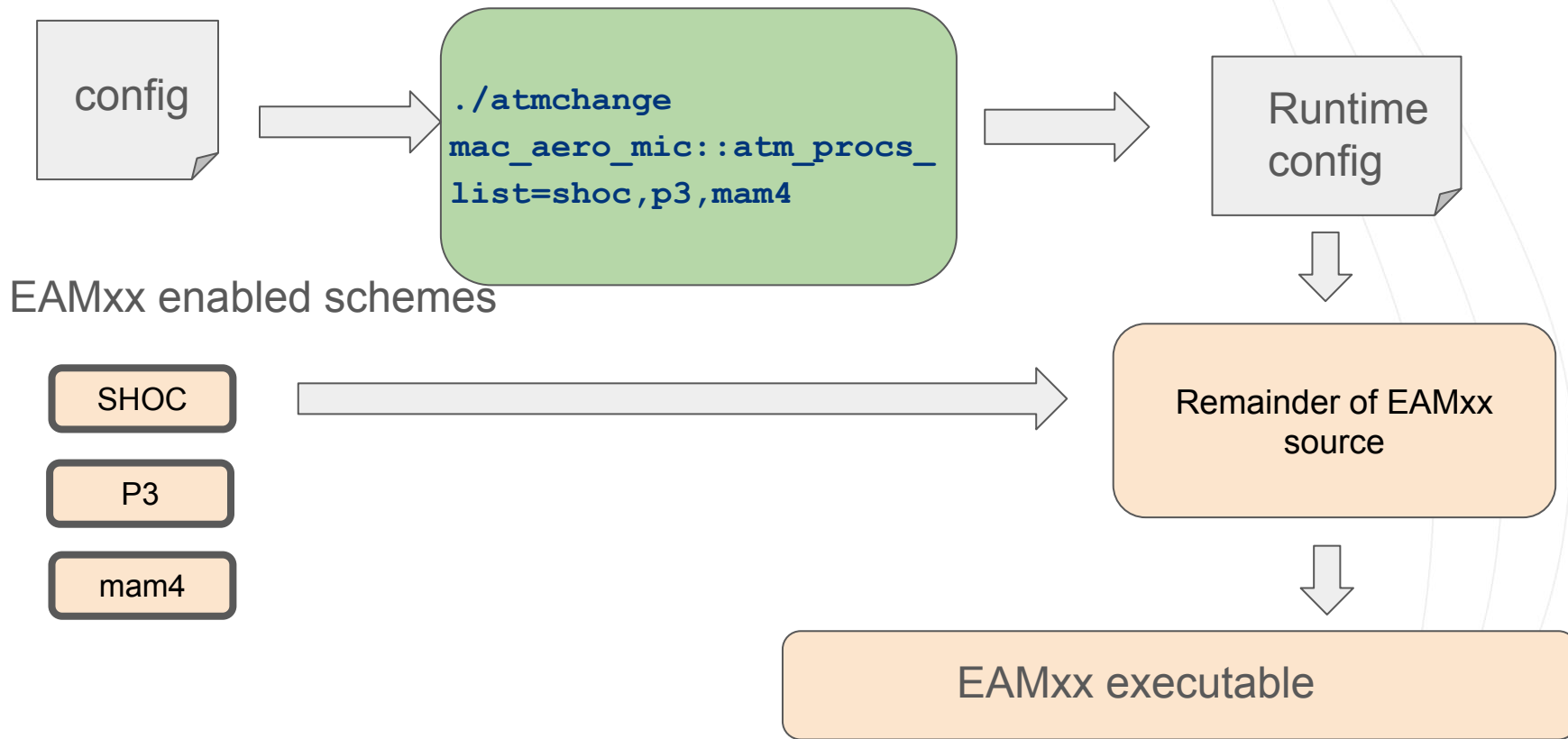
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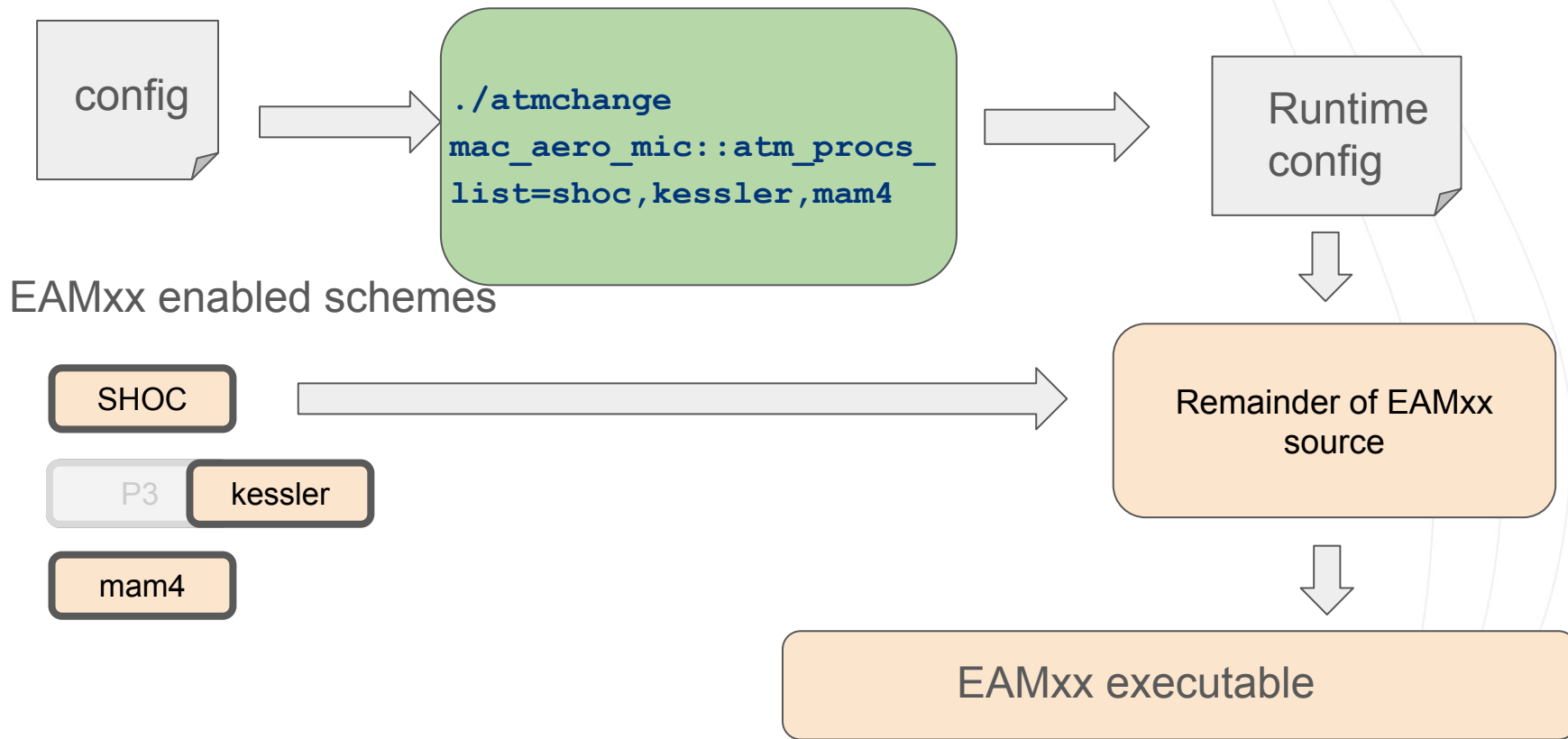
# EAMxx change atmospheric processes



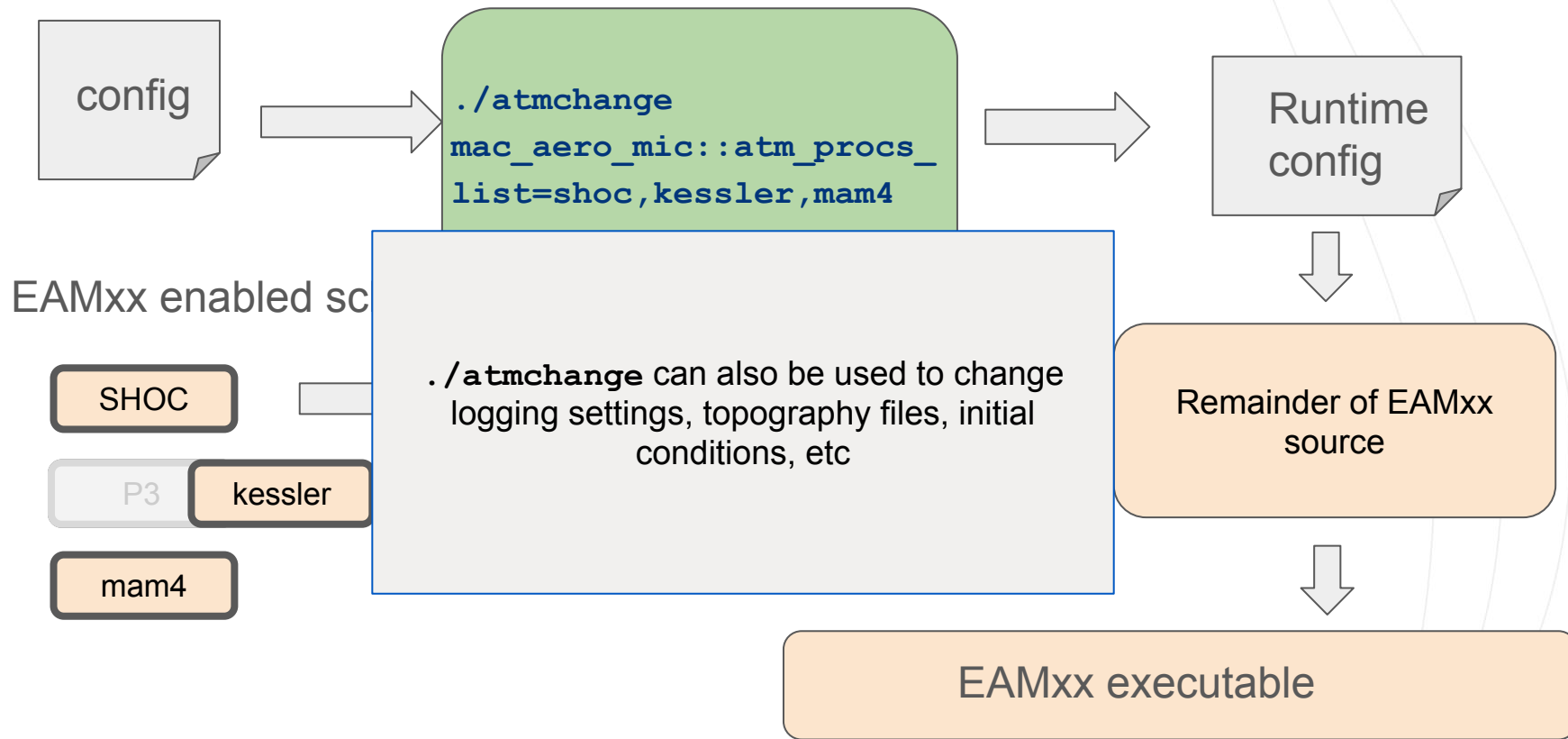
# EAMxx change atmospheric processes



# EAMxx change atmospheric processes



# EAMxx change atmospheric processes



# EAMxx automation & sanity checks



- EAMxx handles grid management & time stepping
- Pre- and post-condition checks for all fields
  - Built-in or user defined checks
  - Embeds domain specific knowledge and improves debuggability
- Automatic data handling
  - File IO
  - Data field management between processes

```
Property check 'precip_liq_surf_mass lower bound check: 0' result: Pass
Property check 'precip_ice_surf_mass lower bound check: 0' result: Pass
Property check 'eff_radius_qc within interval [0, 100]' result: Pass
Property check 'eff_radius_qi within interval [0, 5000]' result: Pass
Property check 'eff_radius_qr within interval [0, 5000]' result: Pass
Property check 'NaN check for field T_mid' result: Pass
Property check 'NaN check for field qv' result: Pass
Property check 'NaN check for field qc' result: Pass
```

# EAMxx parameterization interface overview

- EAMxx parameterizations require the following interface functions:

constructor()

Usually empty

set\_grids()

Define fields  
and grid layout

initialize\_impl()

Create field  
checks  
Initialize things

run\_impl()

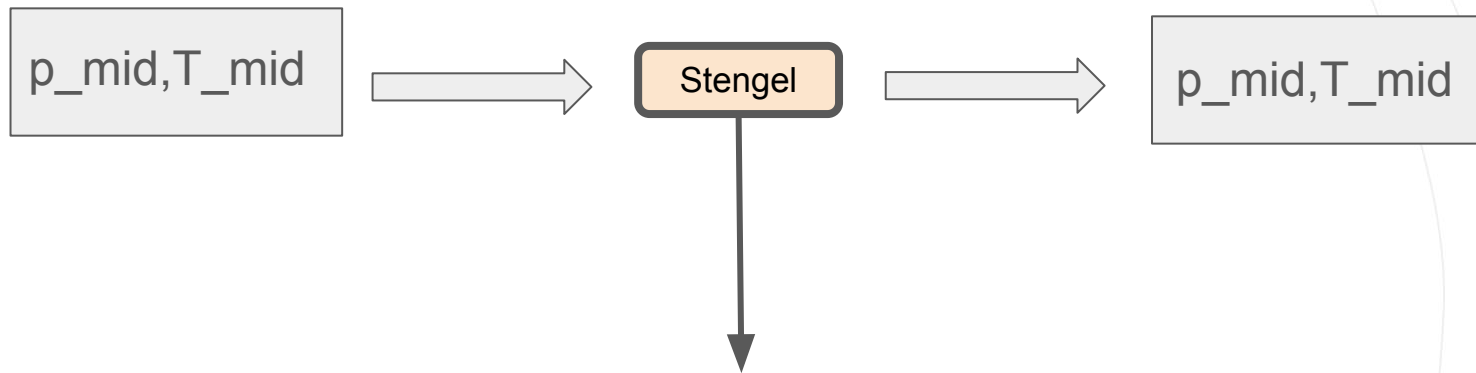
Run physics!

finalize\_impl()

Usually empty

# EAMxx parameterization interface example

- Use an identity transform parameterization as an example



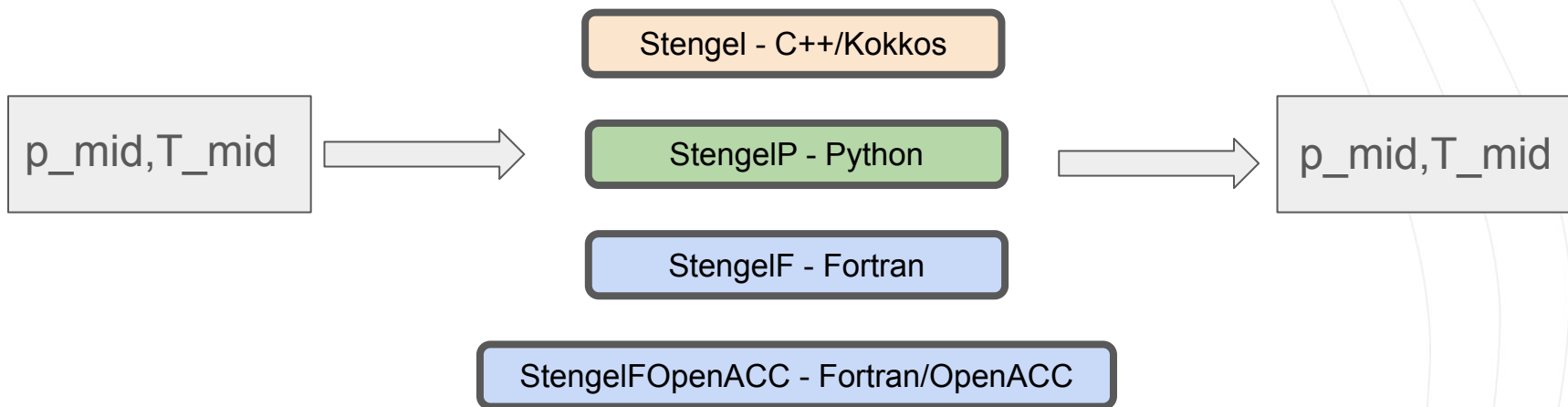
Pressure and temperature at the midpoints ( $p_{\text{mid}}$ ,  $T_{\text{mid}}$ )

$$p_{\text{mid}} = 2 * p_{\text{mid}}; T_{\text{mid}} = 2 * T_{\text{mid}}$$

$$p_{\text{mid}} = 0.5 * p_{\text{mid}}; T_{\text{mid}} = 0.5 * T_{\text{mid}}$$

# EAMxx parameterization interface example

- Use an identity transform parameterization as an example
- Parameterizations can be written with bridges to code in other languages



Pressure and temperature at the midpoints (`p_mid`, `T_mid`)

`p_mid = 2 * p_mid; T_mid = 2 * T_mid`

`p_mid = 0.5 * p_mid; T_mid = 0.5 * T_mid`

# EAMxx parameter interface - C++/Kokkos



## set\_grids()

```
m_grid = gm->get_grid("physics");  
add_field<Updated>("T_mid", ....);  
add_field<Updated>("p_mid", ....);
```

## initialize\_impl()

Nothing to do here.

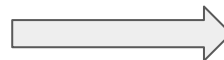
## run\_impl()

```
T_mid = get_field_out("T_mid");  
p_mid = get_field_out("p_mid");  
  
T_mid.scale(2.0);  
p_mid.scale(2.0);  
  
T_mid.scale(0.5);  
p_mid.scale(0.5);
```

p\_mid, T\_mid



Stengel



p\_mid, T\_mid

# EAMxx parameterization interface – Python bridge



## set\_grids()

```
m_grid = gm->get_grid("physics");  
add_field<Updated>("T_mid", .....);  
add_field<Updated>("p_mid", .....);
```

## initialize\_impl()

```
#ifdef EAMXX_HAS_PYTHON  
if (has_py_module()) {  
  try {  
    py_module_call("init");  
  } catch () {  
    // throw error  
  }  
}  
#endif
```

## run\_impl()

```
#ifdef EAMXX_HAS_PYTHON  
T_mid = get_py_field("T_mid");  
p_mid = get_py_field("p_mid");  
if (has_py_module()) {  
  try {  
    py_module_call("main",  
p_mid, T_mid);  
  } catch () {  
    // throw error  
  }  
}  
#endif
```

## stengelP.py

```
def init ():  
  pass  
def main (p_mid, T_mid):  
  p_mid = p_mid * 0.5  
  T_mid = T_mid * 0.5  
  p_mid = p_mid * 2.0  
  T_mid = T_mid * 2.0
```

p\_mid, T\_mid

StengelP

p\_mid, T\_mid

# EAMxx parameter interface - C++ to Fortran bridge



## set\_grids()

```
m_grid = gm->get_grid("physics");  
add_field<Updated>("T_mid", ....);  
add_field<Updated>("p_mid", ....);
```

```
fortran_bridge/  
stengelf_main.F90  
stengelf_bridge.cpp  
stengelf_bridge.hpp
```

## initialize\_impl()

```
stengelf_bridge_init(cols, levs);
```

```
stengelf_bridge_init_c(cols, levs);
```

Calls to fortran init function

## run\_impl()

```
T_mid = get_field_out("T_mid");  
p_mid = get_field_out("p_mid");
```

```
stengelf_bridge_run(cols, levs,  
p_mid, T_mid);
```

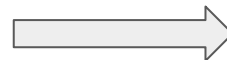
```
stengelf_bridge_run_c(cols, levs,  
p_mid.T, T_mid.T);
```

Calls to fortran run function to do scaling on p\_mid and T\_mid

p\_mid, T\_mid



Stengelf



p\_mid, T\_mid

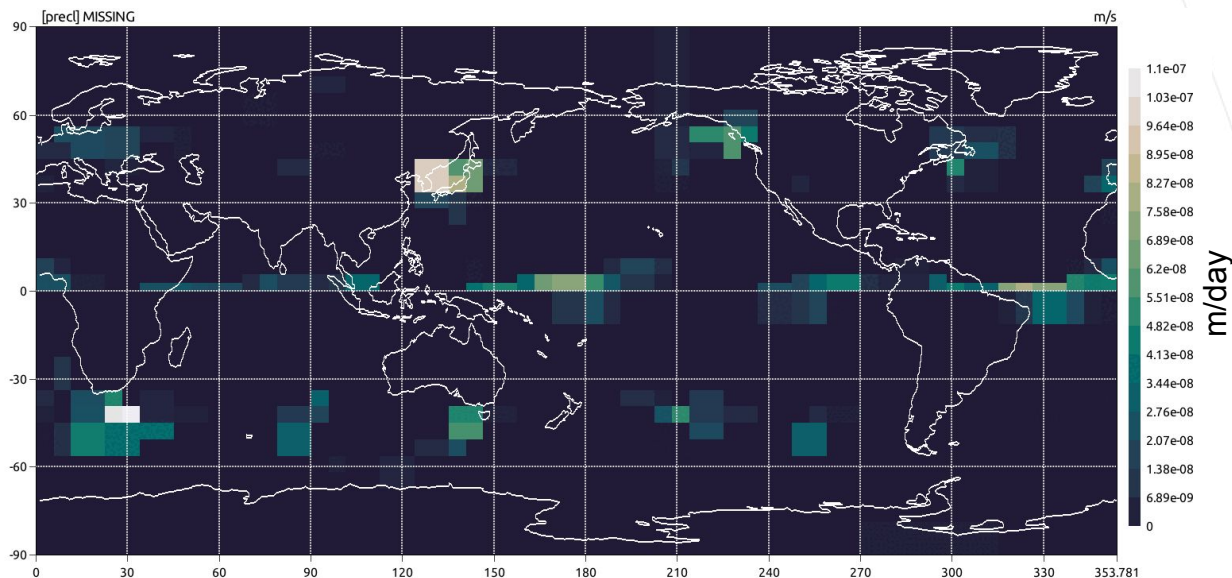
# EAMxx parameterization interface bridges

- C++ and Fortran have different data layouts
  - Requires doing a transpose on fields before going to/from Fortran
  - Use a struct to keep track of C++ and Fortran data fields
- Supports using OpenACC Fortran directives
  - Both the C++ and Fortran code then runs on GPU instead of transferring to CPU for Fortran
- Can bridge directly to existing code from other repositories! (i.e. CLUBB, PUMAS)



- Kessler from CAM-SIMA
  - Small microphysics parameterization (~783 lines, including meta)
  - CCPP generated code: O(1000s) lines
- EAMxx bridge code written:
  - 1202 lines of C++, including debugging code and comments
  - 179 lines of Fortran for bridge
- Time spent:
  - 2 months for all three Stengel\* parameterizations (technical plumbing)
  - Around 2 months for Kessler code
    - I am not a domain expert -> spent a lot of time confused about matching variables, etc
    - Code is currently functional\*

- Verify Kessler in EAMxx versus FKESLER in StormSPEED
  - Requires adding analytical conditions capabilities to EAMxx to run the Kessler simulations



# Next steps



- Verify Kessler in EAMxx versus FKESLER in StormSPEED
  - Requires adding analytical conditions capabilities to EAMxx to run the Kessler simulations
- Additional CAM physics parameterizations in EAMxx framework
  - CLUBB
  - PUMAS
- Explore additional language bridge functionality
  - Python/JAX
  - Rust
  - Julia
- Automating bridge code generation

# Next steps – portability & performance



- Finish GPU enabling Kessler using OpenACC directives
- Compare memory footprint for EAMxx w/Kessler versus FKESLER
- Compare memory footprint & transfers and performance for EAMxx Kessler on CPU, CPU/GPU, and GPU

# Questions?



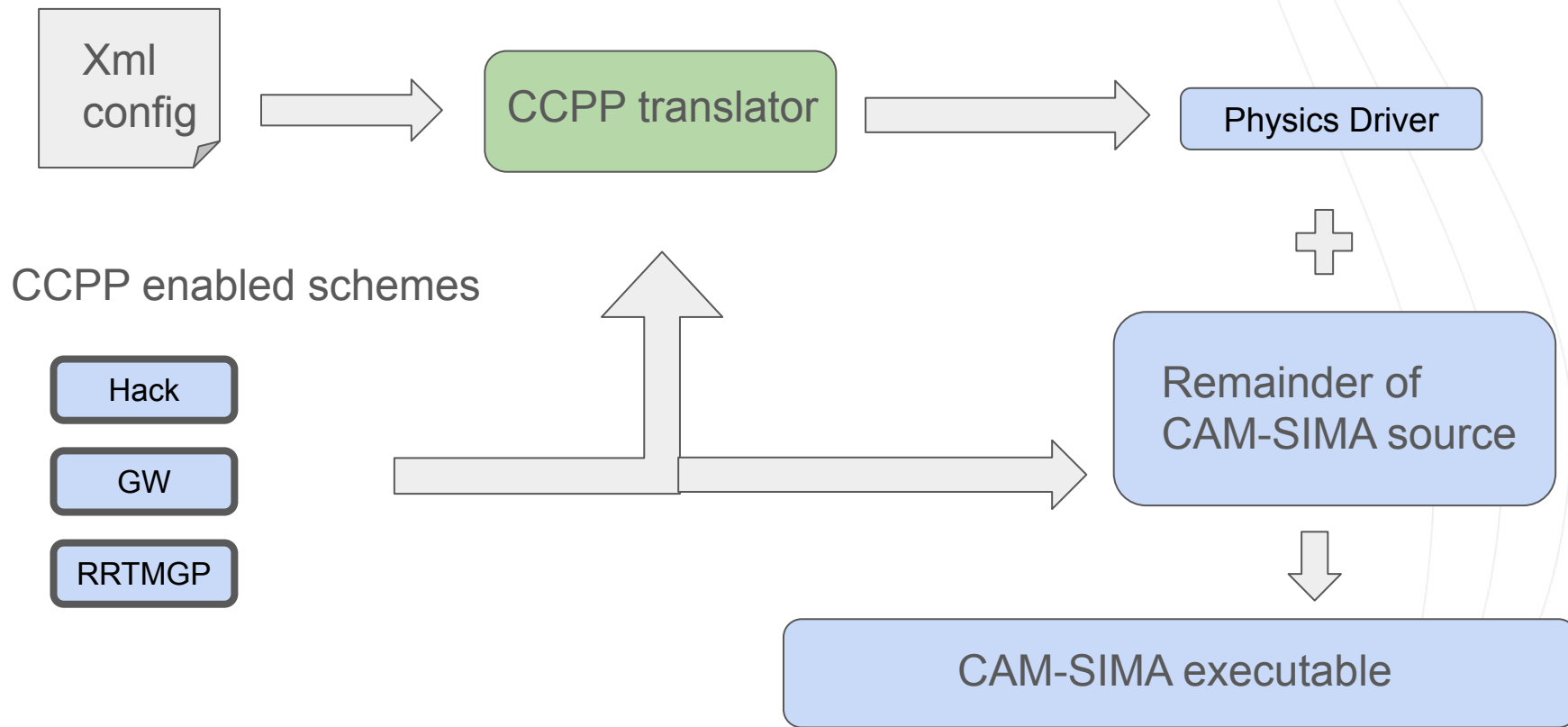
Contact: [kstengel@ucar.edu](mailto:kstengel@ucar.edu)

[Github branch for the Stengel\\* example parameters](#)

\*Contains Stengel (C++ only), StengelF (Fortran w/OpenACC support), and StengelP (Python) as subdirectories

**Supported through the Community Software Facility (CSF)**

# CAM-SIMA change atmospheric processes



# EAMxx parameter interface - C++ to python bridge



## set\_grids()

```
m_grid = gm->get_grid("physics");  
add_field<Updated>("T_mid", ....);  
add_field<Updated>("p_mid", ....);
```

## stengelP.py

```
def init ():  
    pass  
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    p_mid = p_mid * 2.0  
    T_mid = T_mid * 2.0
```

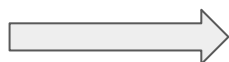
## initialize\_impl()

```
#ifdef EAMXX_HAS_PYTHON  
if (has_py_module()) {  
    try {  
        py_module_call("init");  
    } catch () {  
        // throw error  
    }  
}  
#endif
```

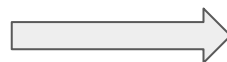
## run\_impl()

```
#ifdef EAMXX_HAS_PYTHON  
T_mid = get_py_field("T_mid");  
p_mid = get_py_field("p_mid");  
if (has_py_module()) {  
    try {  
        py_module_call("main",  
            p_mid, T_mid);  
    } catch () {  
        // throw error  
    }  
}  
#endif
```

p\_mid, T\_mid



StengelP



p\_mid, T\_mid

# EAMxx parameter interface - C++ to python bridge



## set\_grids()

```
m_grid = gm->get_grid("physics");  
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```

## initialize\_impl()

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    T_mid = T_mid * 0.5  
    p_mid = p_mid * 2.0  
    T_mid = T_mid * 2.0
```

p\_mid, T\_mid

StengelP

p\_mid, T\_mid

# EAMxx with Kessler – GPU results



- Put in CPU and GPU figures if we have them; would want CPU only, CPU/GPU, and all on GPU if possible. Want to show matching results between the three

# EAMxx change atmospheric process settings



- Use the `./atmchange` functionality to change atmospheric process settings at runtime:
  - Change logging levels:
    - `./atmchange atm_log_level=debug`
  - Change overall physics processes:
    - `./atmchange physics::atm_procs_list=mac_aero_mic,rrtmgp`
  - Change the parameterizations & their ordering:
    - `./atmchange mac_aero_mic::atm_procs_list=shoc,cld_fraction,spa,kessler`
    - `./atmchange mac_aero_mic::atm_procs_list=shoc,cld_fraction,spa,mam4_aci,p3`
- Can also be used to set topography file or change initial conditions, etc

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