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Progress in implementing GEOS-Chem within CESM

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Agenda

1. Motivation
2. Progress
3. Challenges
4. Next steps

Motivation

CESM - GC: Development guideline

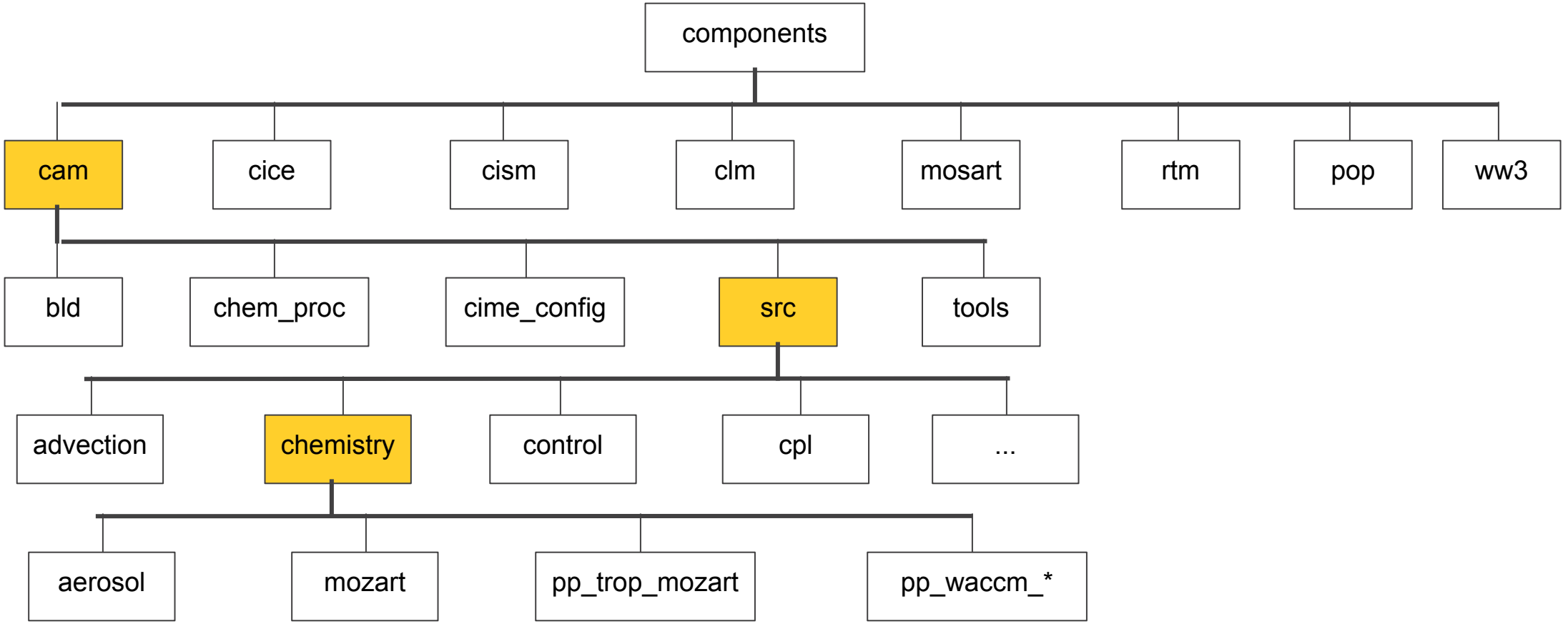
Goal

Global GEOS-Chem simulations with GCM capabilities (online meteorology, ...)

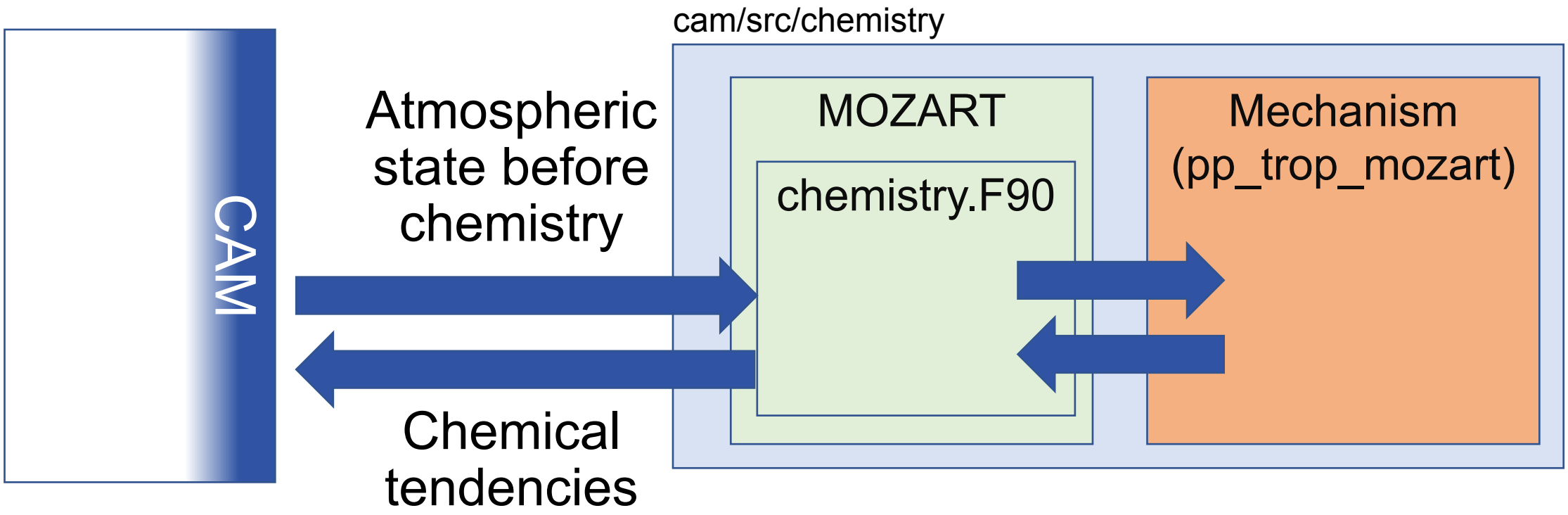
Development guideline

Using GEOS-Chem chemistry module while benefiting of CESM **massively parallel architectures** for high performance, similar to WRF, GCHP, ...

Architecture

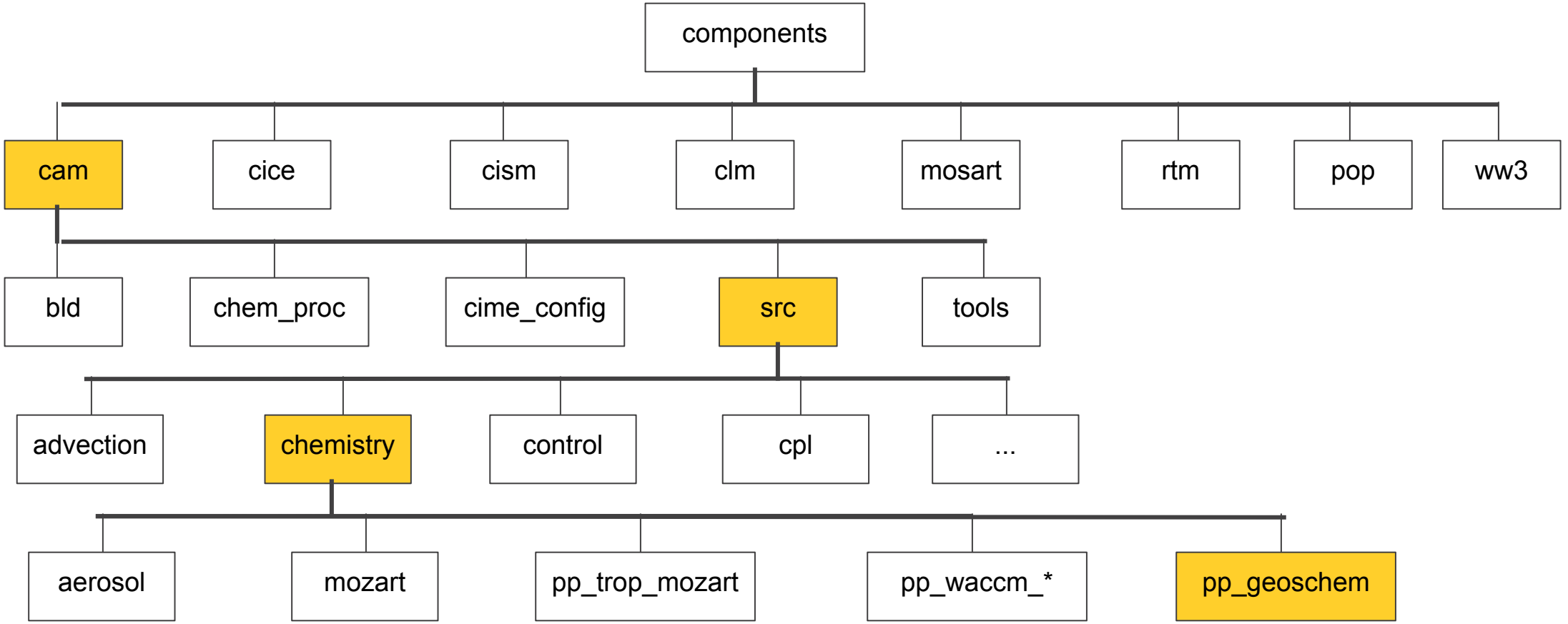


CAM ↔ CAM-Chem chemistry interface

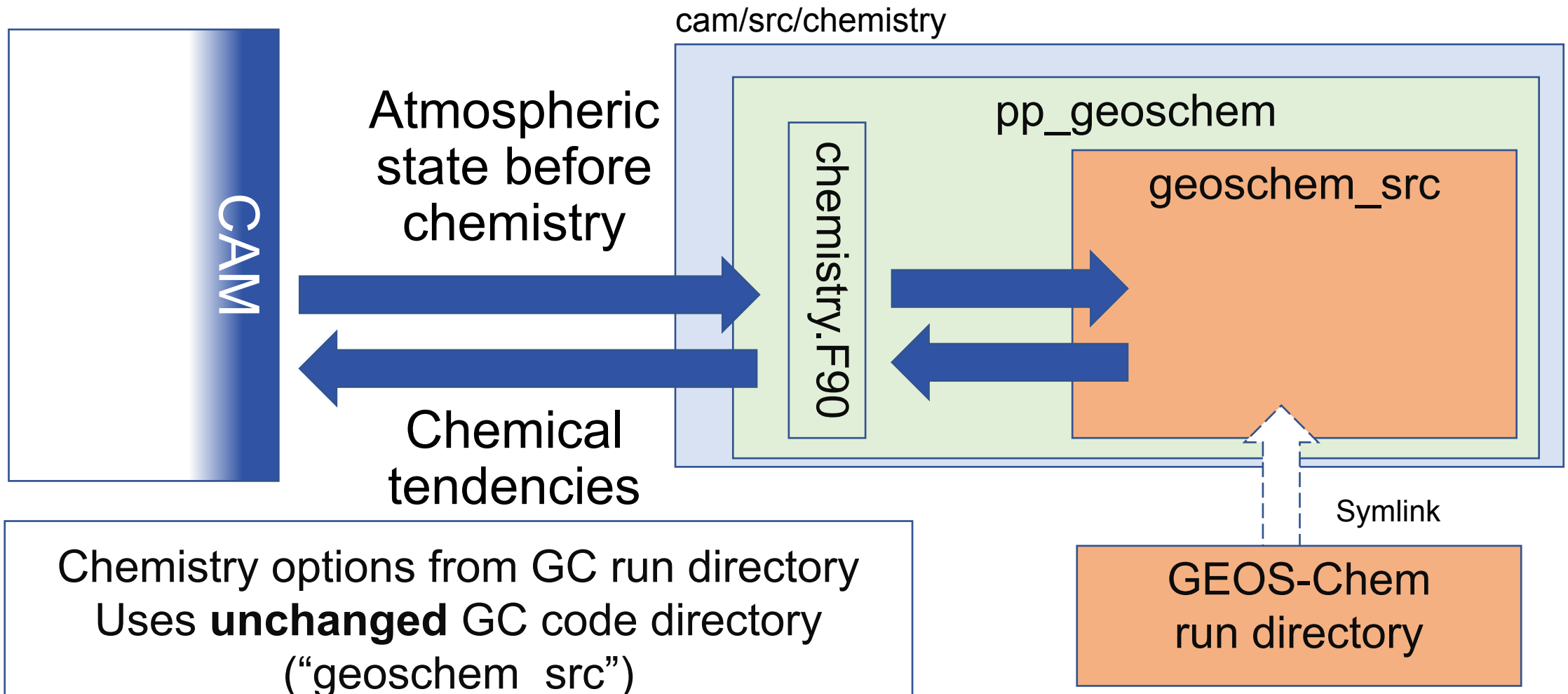


Chemistry options set through CESM
Uses the MOZART interface with multiple mechanisms

Proposed architecture of CESM-GC



CAM ↔ GEOS-Chem chemistry interface



Chemistry options from GC run directory
Uses **unchanged** GC code directory ("geoschem_src")

Progress

Structure of `pp_geoschem`

```
drwxr-xr-x  2 tfritz jacob_lab  540 Jan  6 09:35 ./
drwxr-xr-x 24 tfritz jacob_lab  681 Nov  6 10:31 ../
-rw-r--r--  1 tfritz jacob_lab  47K Nov  6 13:25 aero_model.F90
-rw-r--r--  1 tfritz jacob_lab 6.9K Nov 10 21:02 charge_neutrality.F90
-rw-r--r--  1 tfritz jacob_lab  91K Jan  3 23:14 chemistry.F90
-rw-r--r--  1 tfritz jacob_lab 3.8K Nov 21 17:12 chem_mods.F90
-rw-r--r--  1 tfritz jacob_lab 1.3K Nov 10 21:04 chem_prod_loss_diags.F90
-rw-r--r--  1 tfritz jacob_lab 5.5K Nov 10 21:09 clybry_fam.F90
-rw-r--r--  1 tfritz jacob_lab  19K Nov 10 21:17 epp_ionization.F90
-rw-r--r--  1 tfritz jacob_lab  798 Nov 20 12:57 .exclude
-rw-r--r--  1 tfritz jacob_lab 2.3K Nov 21 17:40 gc_emissions.F90
lrwxrwxrwx  1 tfritz jacob_lab   30 Nov 14 15:54 geoschem_src -> /n/home10/tfritz/CESM2-GC_Src/
-rw-r--r--  1 tfritz jacob_lab  13K Nov 12 12:57 mo_apex.F90
-rw-r--r--  1 tfritz jacob_lab  54K Nov 10 21:32 mo_gas_phase_chemdr.F90
-rw-r--r--  1 tfritz jacob_lab 7.9K Nov 10 21:37 mo_lightning.F90
-rw-r--r--  1 tfritz jacob_lab 5.9K Nov 12 11:51 rate_diags.F90
-rw-r--r--  1 tfritz jacob_lab 7.3K Nov 21 14:41 short_lived_species.F90
-rw-r--r--  1 tfritz jacob_lab  11K Nov 12 13:14 upper_bc.F90
```

- Interface with GEOS-Chem through `**chemistry.F90**`
- Symbolic link to almost **unmodified GEOS-Chem source folder**
- `**.exclude**` file to only compile required GEOS-Chem file

Compiling - Excluding unnecessary GEOS-Chem files

Changes to `scripts/Tools/mkSrcfiles`:

```
    @filenames = (glob("$dir/*.[Ffc]"), glob("$dir/*.[Ff]90"), glob("$dir/*.cpp"));
    foreach $filename (@filenames) {
        $filename =~ s!.*/!!;                   # remove part before last slash
        if (defined $skip_prefix){
            if ($filename =~ /^${skip_prefix}/){
            print "WARNING: Skipping file $dir/$filename Source files beginning in $skip_prefix are
↪ ignored\n";
            next;
            }
        }
        # If filename is in local exclude file, don't add to list.
        if ($useExclude) {
            my $matches = grep { /$filename/ } @excludes;
            if ($matches) {
                print "Exclusion matched file, $filename in $dir\n\n";
            }else{
                $src{$filename} = 1;
            }
        }else{
            $src{$filename} = 1;
        }
    }
```

As of right now, we just exclude any unnecessary file by reading `.exclude` directly in `scripts/Tools/mkSrcfiles`.

Compiling - Passing GEOS-Chem flags to compile command

Changes to `cam/bld/configure`:

```
# TMMF - wedge in GEOS-Chem CPP definitions here
if ($chem_pkg =~ 'geoschem') {
    $chem_cppdefs .= ' -DEXTERNAL_GRID -DEXTERNAL_FORCING -DUCX -DMERRA2 -DLINUX_IFORT -
↪DUSE_REAL8 -DMODEL_CESM';
    # TMMF - Temporary fix
    $chem_nadv = 200;
}
```

- Passing **GEOS-Chem CPP flags** through CAM's `bld/configure` file
- Passing **MODEL_CESM** CPP flag to GEOS-Chem to hand I/O to CESM (e.g. read *.nc files) and broadcast any data to other tasks.
- File is read at each call of `./case.build`

Compiling - Miscellaneous

Miscellaneous

Other changes to make GEOS-Chem compilable with CESM:

- Defining components
- Defining compsets
  - 2000_CAM40%GC_SLND_SICE_SOCN_SROF_SGLC_SWAV
  - 2000_CAM%GCHS_SLND_SICE_SOCN_SROF_SGLC_SWAV
  - 2000_CAM40%GC_CLM40%SP_CICE%PRES_DOCN%DOM_RTM_SGLC_SWAV

Interface file - chemistry.F90

Interface

Different subroutines:

- **chem_register**
  - register species and defines mapping between species
- **chem_readnl**
  - reads input.geos
- **chem_init**
  - initializes State_Grid, State_Met, State_Chm, State_Diag
  - initializes GEOS-Chem modules
- **chem_timestep_tend**
  - transfers CESM meteorology to State_Met
  - performs any conversion/unit change
  - performs chemistry
- **chem_final**
  - cleanup
- ...

Current status of CESM-GC coupling

Progress

- GEOS-Chem **"Standard" chemistry mechanism** (Trop-strat with "complex" SOA)
- **Fast-JX** photolysis scheme
- Bulk aerosol scheme with **ISORROPIA II equilibrium**
- **Wet scavenging** – no dry deposition or emissions

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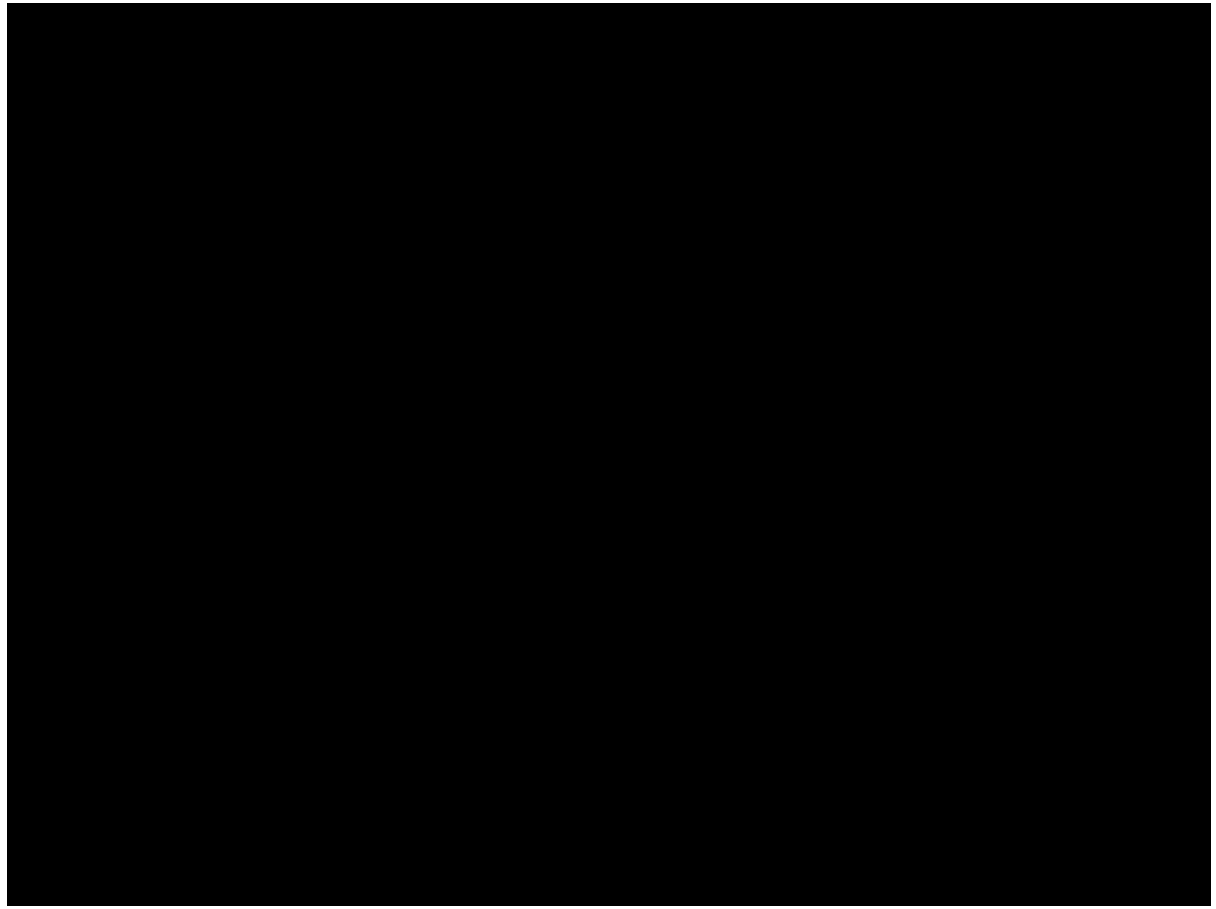
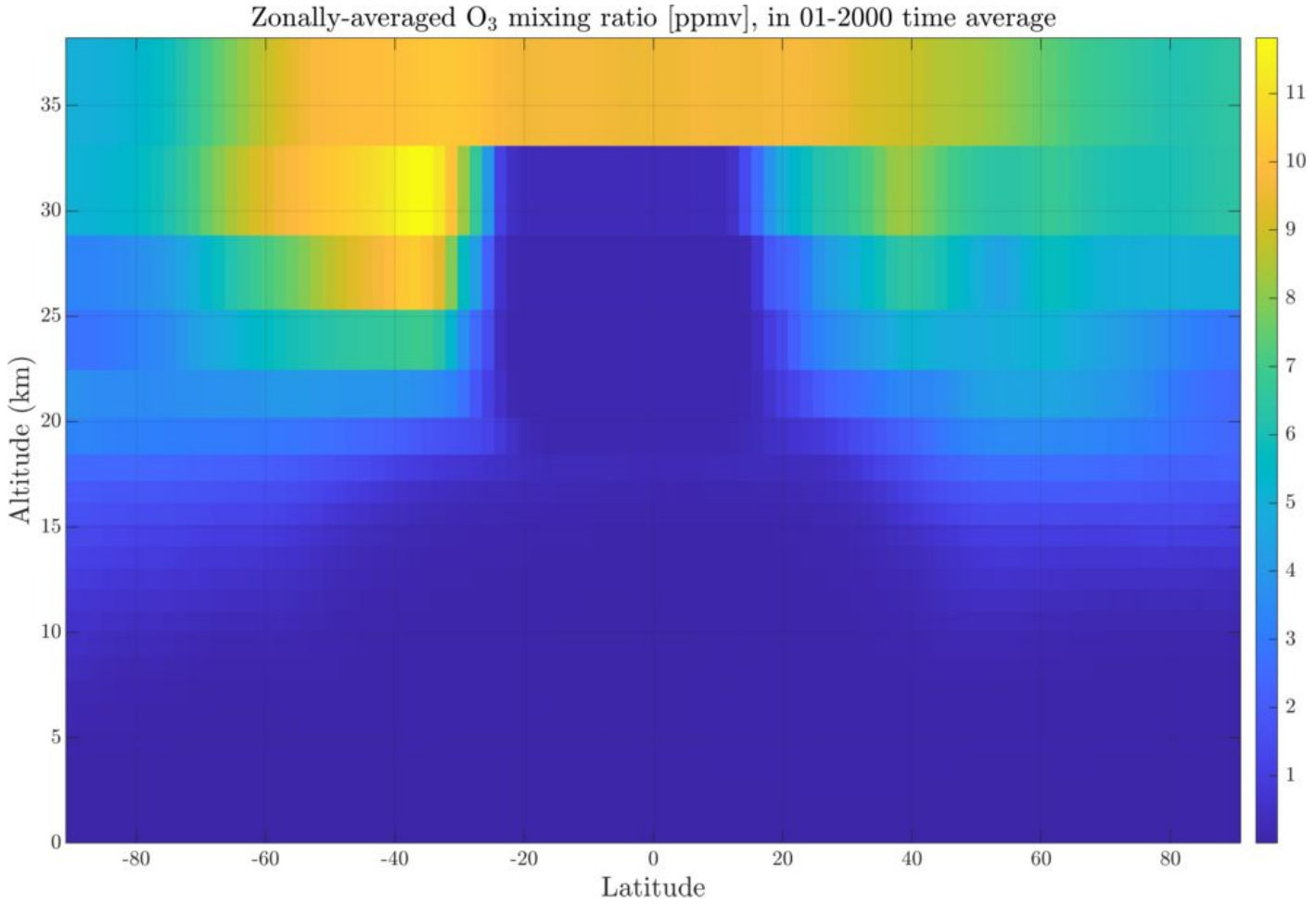


Current status of CESM-GC coupling



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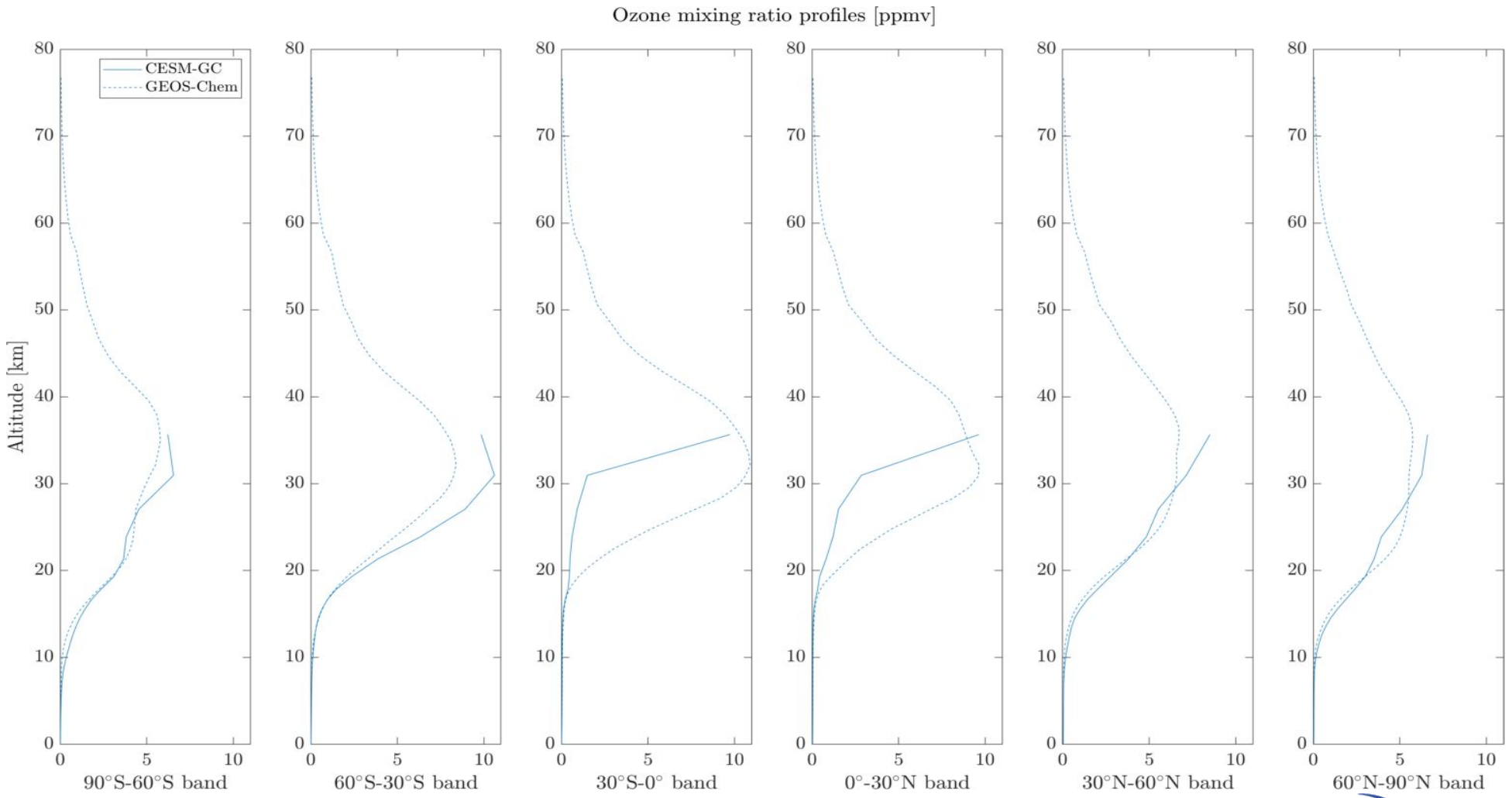

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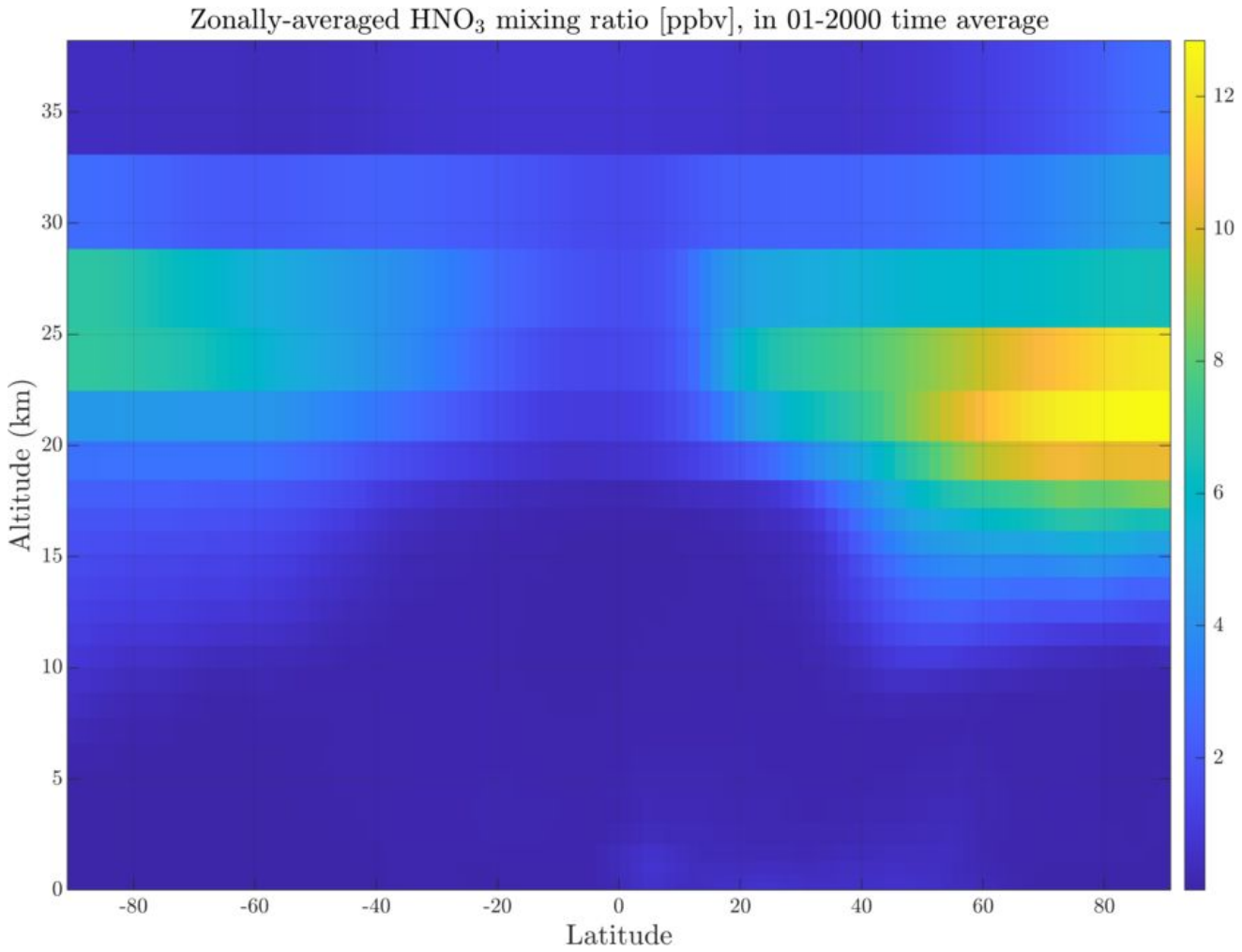

Challenges

CESM-GC coupling - Challenges

Issues

- Grid-independency
  - Making sure that results from CESM-GC are grid-independent
  - Assumptions valid at all resolutions

- Compatibility with CESM development.
  - Only have one version of CESM-GC

CESM-GC coupling - Unresolved issues

Issues

- Interaction between CAM and CLM
  - How would dry deposition make CAM and CLM interact?
- Aerosol representation in CESM vs GEOS-Chem
- Convection / PBL mixing

CESM-GC coupling - Science

Science questions

- Use CESM-GC coupling to have an **intercomparison between GEOS-Chem and CAM-Chem** within CESM (using online meteorology, ...)
- Test cases for **software**?
- Test cases for **science**?
- Merge GEOS-Chem and CESM post-processing tools?

Next steps

Summary and next steps

Summary

- Working prototype of CESM-GC within CESM is available
- Key objective is to **maintain connection to GEOS-Chem main branch**
- Could provide a **two-way channel** for improvements between communities

Questions to resolve

- When should we (not) be chemistry-specific?
- Interface with CAM
  - Convection/PBL mixing
  - Dry deposition
  - Emissions (HEMCO)
  - Aerosols (bulk in GEOS-Chem)
- What should the development goals be (e.g. enabling hybrid OpenMP/MPI?)

At NCAR

Future steps

- Work on improving the current CESM-GC prototype
- Gain deeper understanding of each component (CAM, CLM, ...) and how they interact
- Improve knowledge of MPI and its usage in CESM
- Benefit from CESM-GC coupling to learn from both communities

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