Computing New Diagnostic Fields in MPAS-Atmosphere Simulations

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Motivation

As the number of people using MPAS-Atmosphere increased to even a very modest number, it was recognized that we needed some structured way of introducing the computation of new diagnostics

We wanted a framework that could handle:

- Instantaneous diagnostics

- Cumulative diagnostics

- Extreme value diagnostics

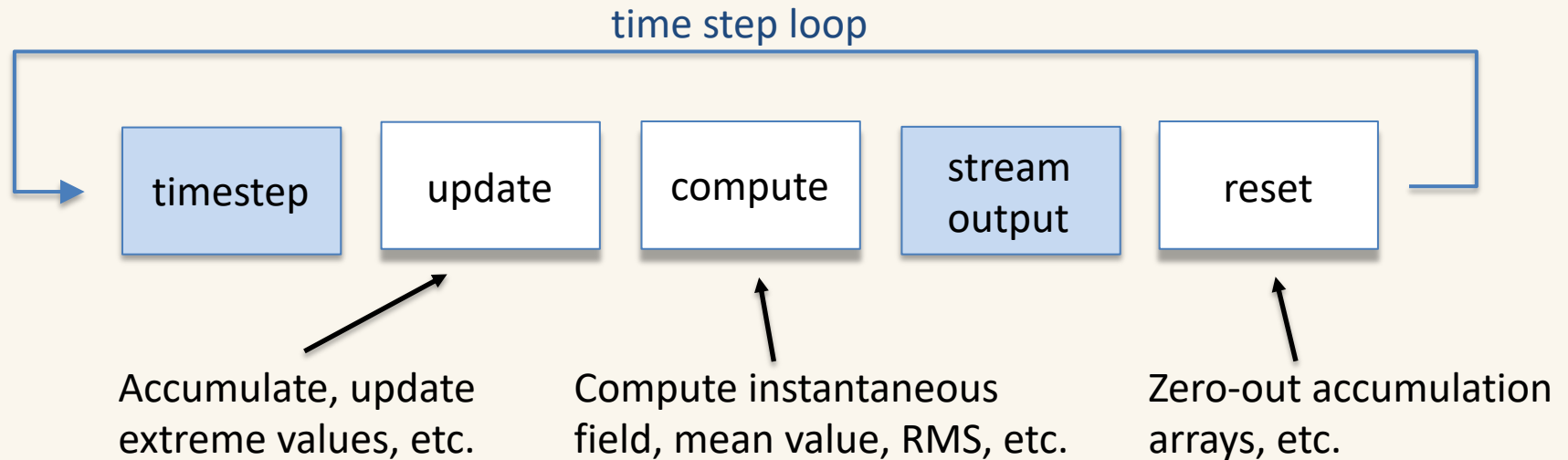- *Or anything that looked like the above from a computational standpoint!*

Diagnostics should be able to change in response to modifications of the streams that write them, too.

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Introduction

Broadly, there are five stages in the computation of diagnostics like those types listed on the previous slide:

1. **Setup –** Pre-allocate arrays that will be needed by the diagnostic during the simulation, initialize values, etc.

2. **Update –** Accumulate values, update extrema, etc.

3. **Compute –** Divide by the accumulation period to get mean values, compute instantaneous fields, etc.

4. **Reset –** After writing the diagnostic, zero-out accumulation arrays, etc.

5. **Cleanup –** Deallocate any memory that was allocated by the diagnostic

Other than *Setup* and *Cleanup*, how do these phases fit into the sequence of a model timestep?

time step loop

| timestep | update | compute | stream output | reset |

Accumulate, update extreme values, etc.

Compute instantaneous field, mean value, RMS, etc.
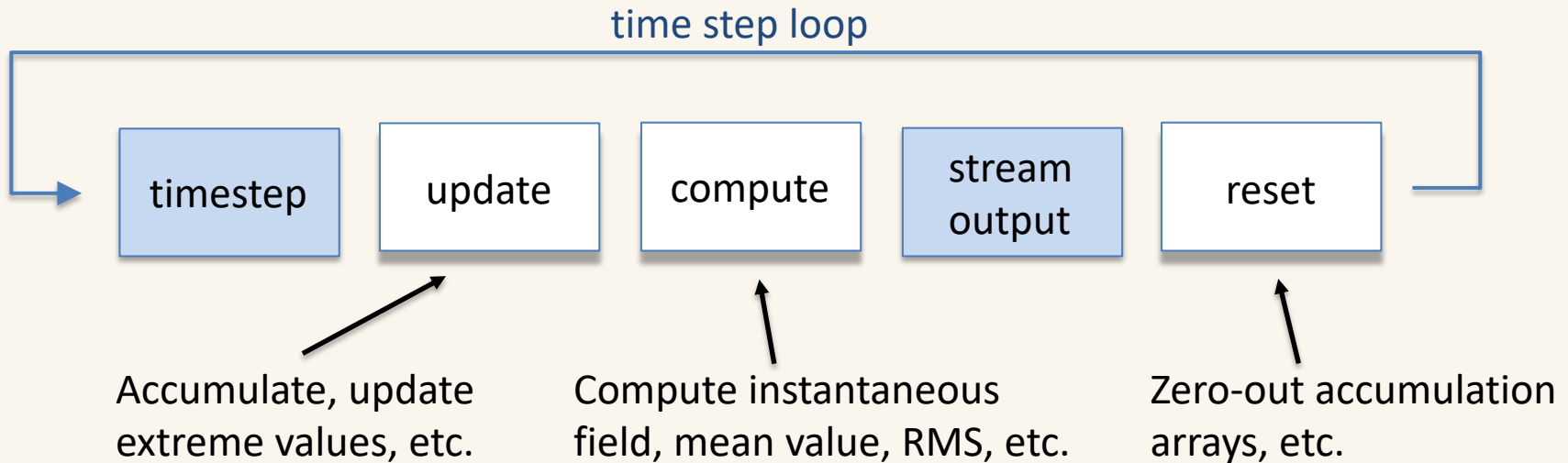
Zero-out accumulation arrays, etc.

Critically, we need some way for a diagnostic to determine whether it will be written out in a given timestep!

Diagnostics utilities

Along with the diagnostics framework, a utility module has been written that will tell a diagnostic:

- Whether its field will be written in a given timestep
  - Generally called from the *Compute* phase
- How many output streams include its field

time step loop

| timestep | update | compute | stream output | reset |

Accumulate, update extreme values, etc.

Compute instantaneous field, mean value, RMS, etc.

Zero-out accumulation arrays, etc.

Code organization

In terms of code structure, where do we add diagnostics?

- The idea is that all diagnostics should be implemented as self-contained modules

- All diagnostics modules should reside in the same place

```
MPAS-Model/
    src/
        core_atmosphere/
            diagnostics/
            dynamics/
            inc/
            physics/
            Registry.xml
            utils/
```

Add new diagnostics in this directory

The main Registry.xml file will include "sub-Registry" sections from the diagnostics directory

Code organization

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```
MPAS-Model/
    src/
        core_atmosphere/
            diagnostics/
                Makefile
                Registry_diagnostics.xml
                mpas_atm_diagnostics_manager.F
            dynamics/
            inc/
            physics/
            Registry.xml
            utils/
```

These files serve as the interface between your new diagnostic and the rest of MPAS

How to add a new diagnostics?

1. Define new namelist options and fields in a new `Registry_<your_diagnostic>.xml` file. Add a `#include` statement for this new Registry section in the `Registry_diagnostics.xml` file.

2. Create a new module for the diagnostic.

3. Add calls to your diagnostic's *setup*, *update*, *compute*, *reset*, and *cleanup* routines in the main diagnostic driver.

4. Update the `Makefile` to compile your new diagnostic module.

The `README` file in the `diagnostics/` subdirectory describes the step-by-step process to adding a new diagnostic

Working in the `src/core_atmosphere/diagnostics/` directory:

1. Define the maximum SWDOWN field in a new `Registry_swdown.xml` file

```xml
<var_struct name="diag_physics" time_levs="1">
        <var name="gsw_max" type="real"
             dimensions="nCells Time"
             units="W m^{-2}"
             description="Maximum surface SW radiation flux"/>
</var_struct>
```

2. Include `Registry_swdown.xml` in `Registry_diagnostics.xml`

```xml
<!-- SW radiation diagnostics -->
#include "Registry_swdown.xml"
```

Working in the `src/core_atmosphere/diagnostics/` directory:

3. Write the *setup*, *update*, and *reset* routines for the diagnostic:

```
subroutine swdown_setup(all_pools)

    type (MPAS_pool_type), pointer :: all_pools

    type (MPAS_pool_type), pointer :: diag_physics

    call mpas_pool_get_subpool(all_pools, 'diag_physics', diag_physics)
    call mpas_pool_get_array(diag_physics, 'gsw', gsw)
    call mpas_pool_get_array(diag_physics, 'gsw_max', gsw_max)

    gsw_max(:) = 0.0

end subroutine swdown_setup
```

*Not shown in the code above is the declaration of gsw and
gsw_max <u>pointers</u> as module variables...*

Working in the `src/core_atmosphere/diagnostics/` directory:

3. Write the *setup*, *update*, and *reset* routines for the diagnostic:

```fortran
subroutine swdown_update()

    gsw_max(:) = max(gsw_max(:), gsw(:))

end subroutine swdown_update
```

Working in the `src/core_atmosphere/diagnostics/` directory:

3. Write the *setup*, *update*, and *reset* routines for the diagnostic:

```
subroutine swdown_reset()

   use mpas_atm_diagnostics_utils, only : mpas_field_will_be_written

    if (mpas_field_will_be_written('gsw_max')) then
       gsw_max(:) = 0.0
    end if

end subroutine swdown_reset
```

After adding a couple of lines to the `Makefile`, we're ready to compile MPAS-Atmosphere and try out our new diagnostic

We'll test it by:

- Outputting the gsw_max field every 60 minutes
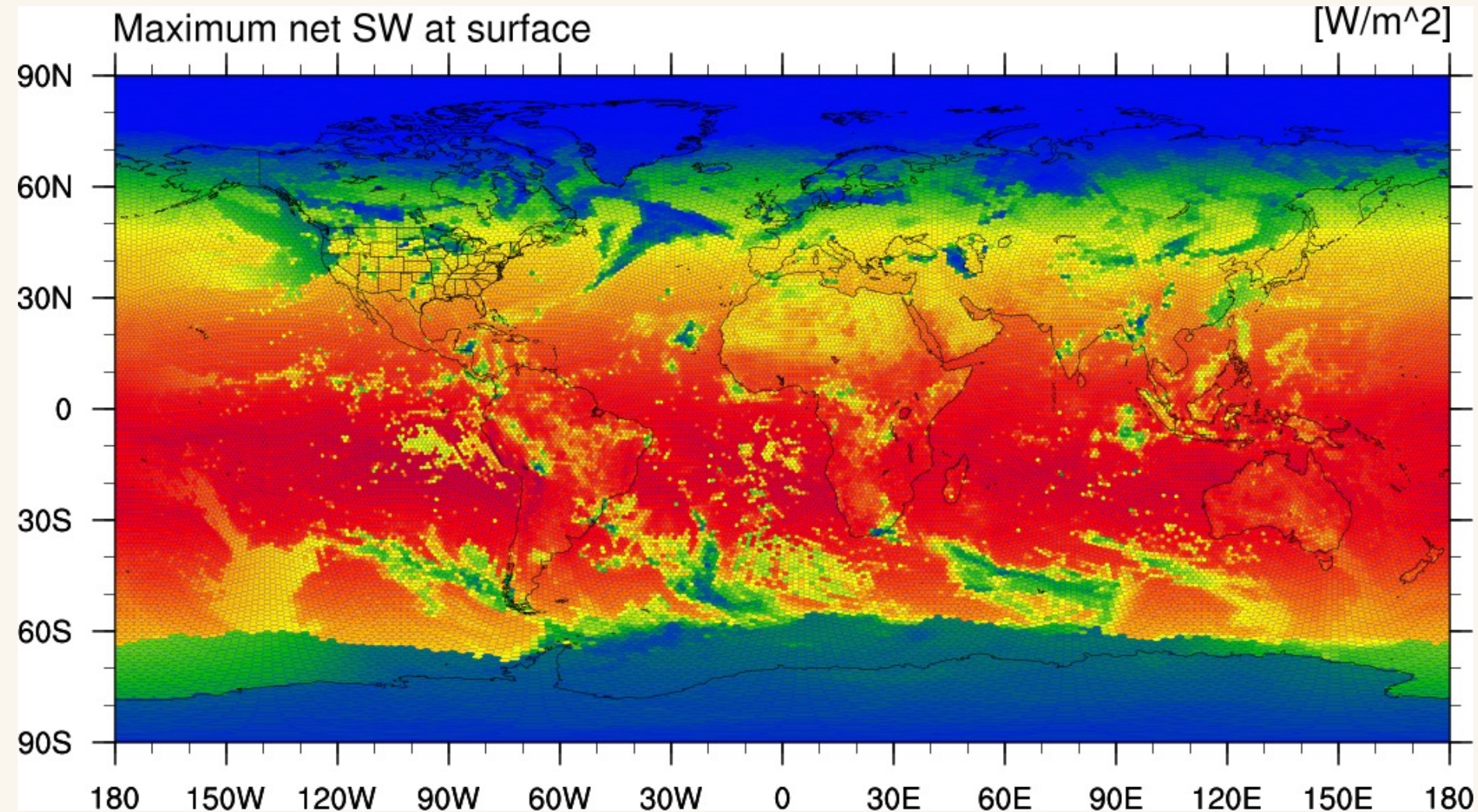
- Outputting the gsw_max field every 1440 minutes

Our test simulation will start at 2010-10-23 at 00 UTC, and we'll look at the output that we get at 2010-10-24 at 00 UTC…

Maximum net SW at surface [W/m^2]

Conclusion
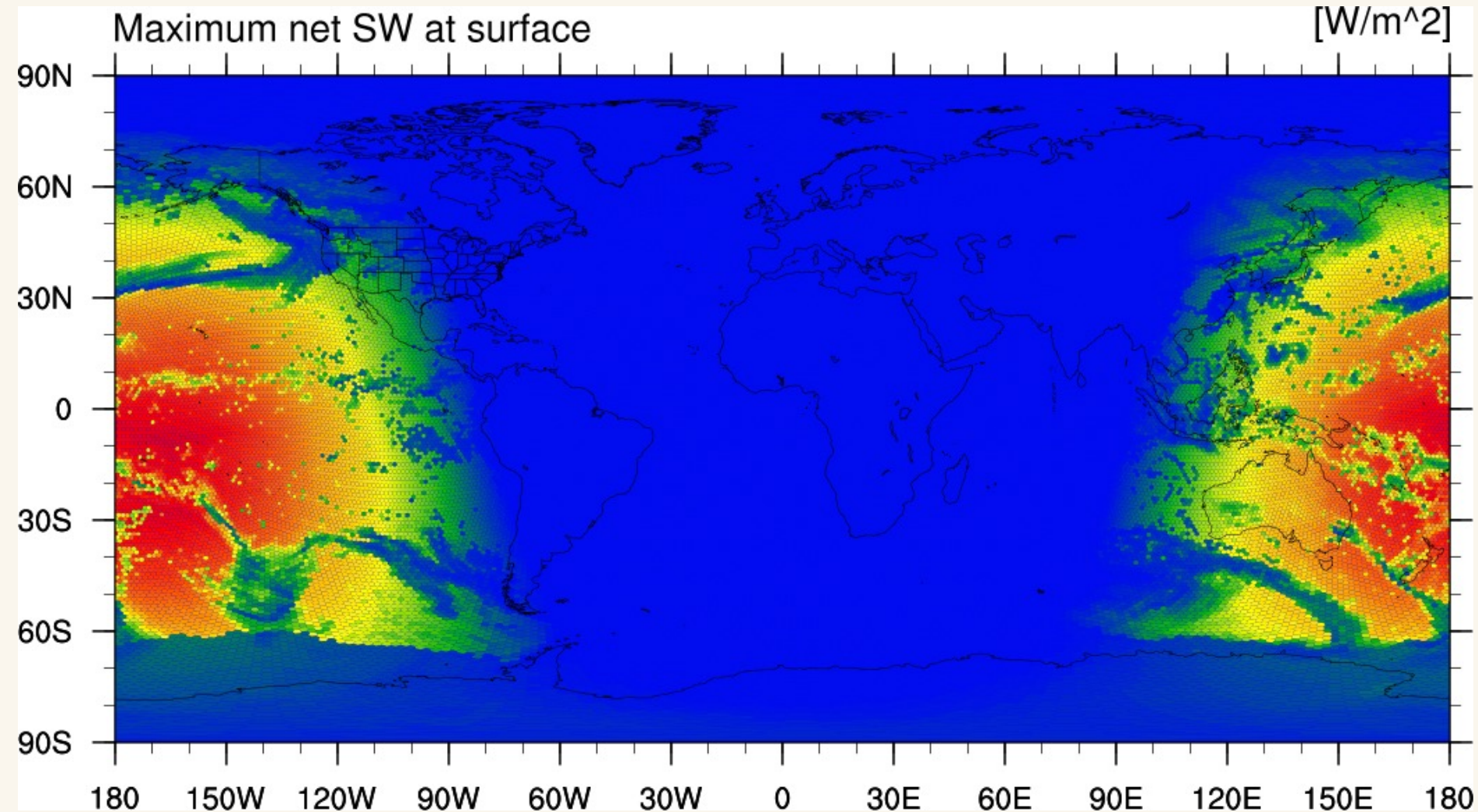
MPAS-Atmosphere provides a framework that enables many types of diagnostic fields to be implemented in a modular way

The file
`MPAS-Model/src/core_atmosphere/diagnostics/README`
summarizes the steps to implementing a new diagnostic.