National Aeronautics and Space Administration

Encapsulating the Aerosol State for Modeling, Data Assimilation and 1D-Var Retrievals

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Outline

- Interoperability, shmoperability
- Diversity of aerosol states
- Typical model physics interface
- Data Assimilation Interfaces
  - Aerosol observables
  - Generic Observation Operators
- Proposal for Community Exercise

Interoperability

What do you mean by interoperability?

Interoperability is the real-time data exchange between different systems that speak directly to one another in the same language, instantly interpreting incoming data and presenting it as it was received while preserving its original context.

Interoperability of Aerosol Related Software

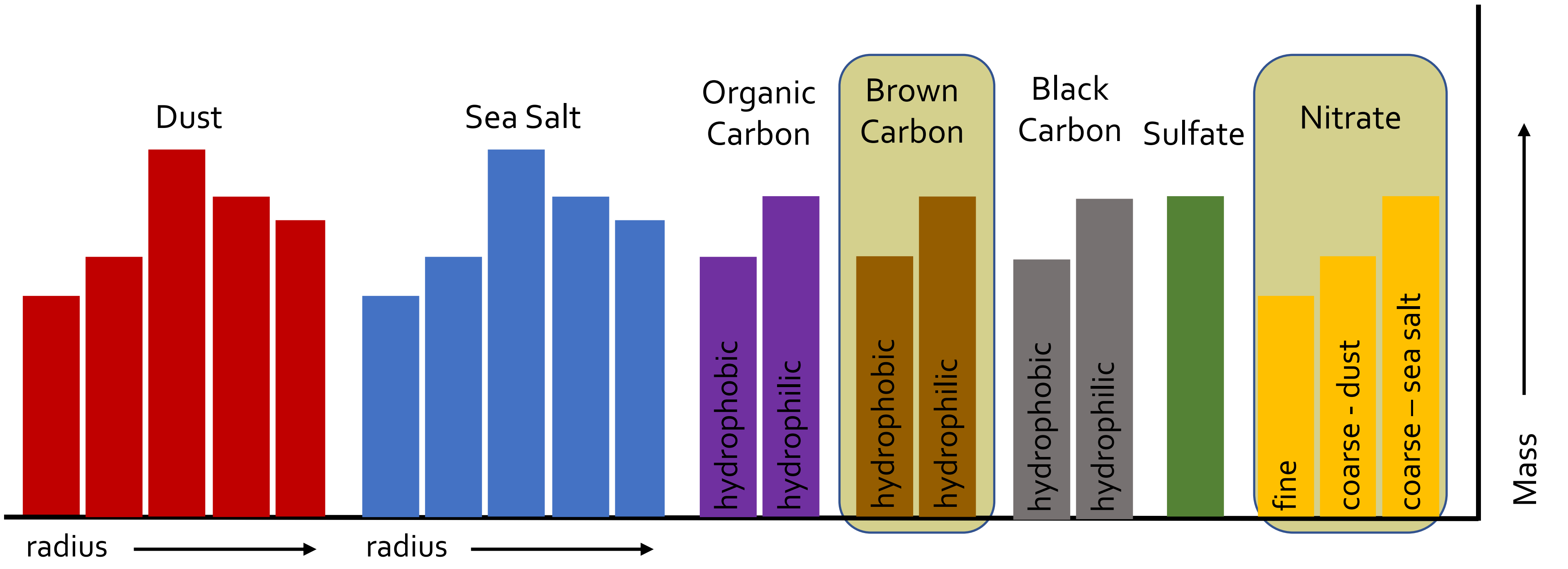
- Although it has its merits, and in many ways can simplify the construction of interoperable components, let's ignore for now
  - File formats
  - Metadata conventions
- Let's focus instead on the *Aerosol State* and the functionality it must provide for
  - Interfacing to model physics (radiation, gas chemistry and cloud microphysics)
  - Simulate aerosol related *Observables* by means of generic observation operators
  - And eventually generic data assimilation functionality (domain of JEDI)
- Key principles to adhere to:
  - Separation of concerns
  - Know on a need-to-know basis
  - Overall consistency throughout the earth system model and data assimilation systems

Examples of Aerosol States

Gases are molecules, aerosols come in all shapes, forms, and sizes

- Bulk schemes
- Modal Schemes
- Sectional Schemes

GOCART-2G: Bulk, Sectional-ish Component in GEOS



7-mode Modal Aerosol Module Configuration in GEOS

Aitken

number
water
sulfate
ammonium
secondary OM
sea salt

$\sigma=1.6$

coagulation and condensation

Accumulation

number
water
sulfate
ammonium
secondary OM
hydrophobic OM
black carbon
sea salt

$\sigma=1.8$

Fine Dust

number
water
dust
sulfate
ammonium

a	c
du_a_fdu	du_c_fdu
su_a_fdu	su_c_fdu
amm_a_fdu	amm_c_fdu

$\sigma=1.8$

Fine Sea Salt

number
water
sea salt
sulfate
ammonium

$\sigma=2.0$

aged to the accumulation mode due to condensation of H2SO4, NH3 and SOA(gas)

Primary Carbon

number
water
hydrophobic OM
black carbon

$\sigma=1.6$

Coarse Dust

number
water
dust
sulfate
ammonium

$\sigma=1.8$

Coarse Sea Salt

number
water
sea salt
sulfate
ammonium

$\sigma=2.0$

Two attachment states:

a) ***interstitial*** *- suspended in (clear or cloudy) air*

b) ***cloud-borne*** *- attached to / contained within stratiform cloud droplets (AP in convective cloud droplet are not treated explicitly)*

Sectional Schemes: CARMA

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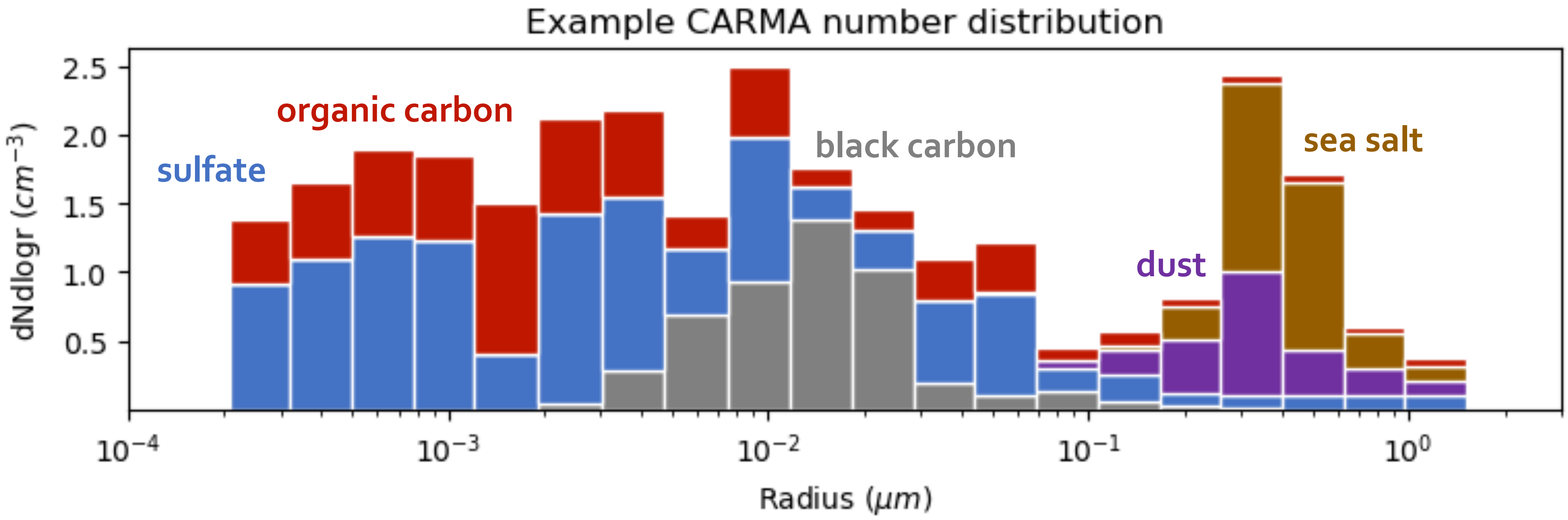
- CARMA tracks a sectional aerosol size distribution separated into a configurable number of size bins
- Calculates microphysical processes (nucleation, condensation/evaporation, coagulation, settling) to update the size distribution
- Configurable to track multiple aerosol elements (i.e., species) in each internally mixed groups
- Has been coupled to both GEOS-Chem and GMI sulfur chemistry
- Dynamic aerosol optical properties calculated using lookup tables → currently coupled to inline radiative transfer for direct effect, working on coupling to photolysis
- Provides dynamic surface area for calculation of heterogeneous chemistry

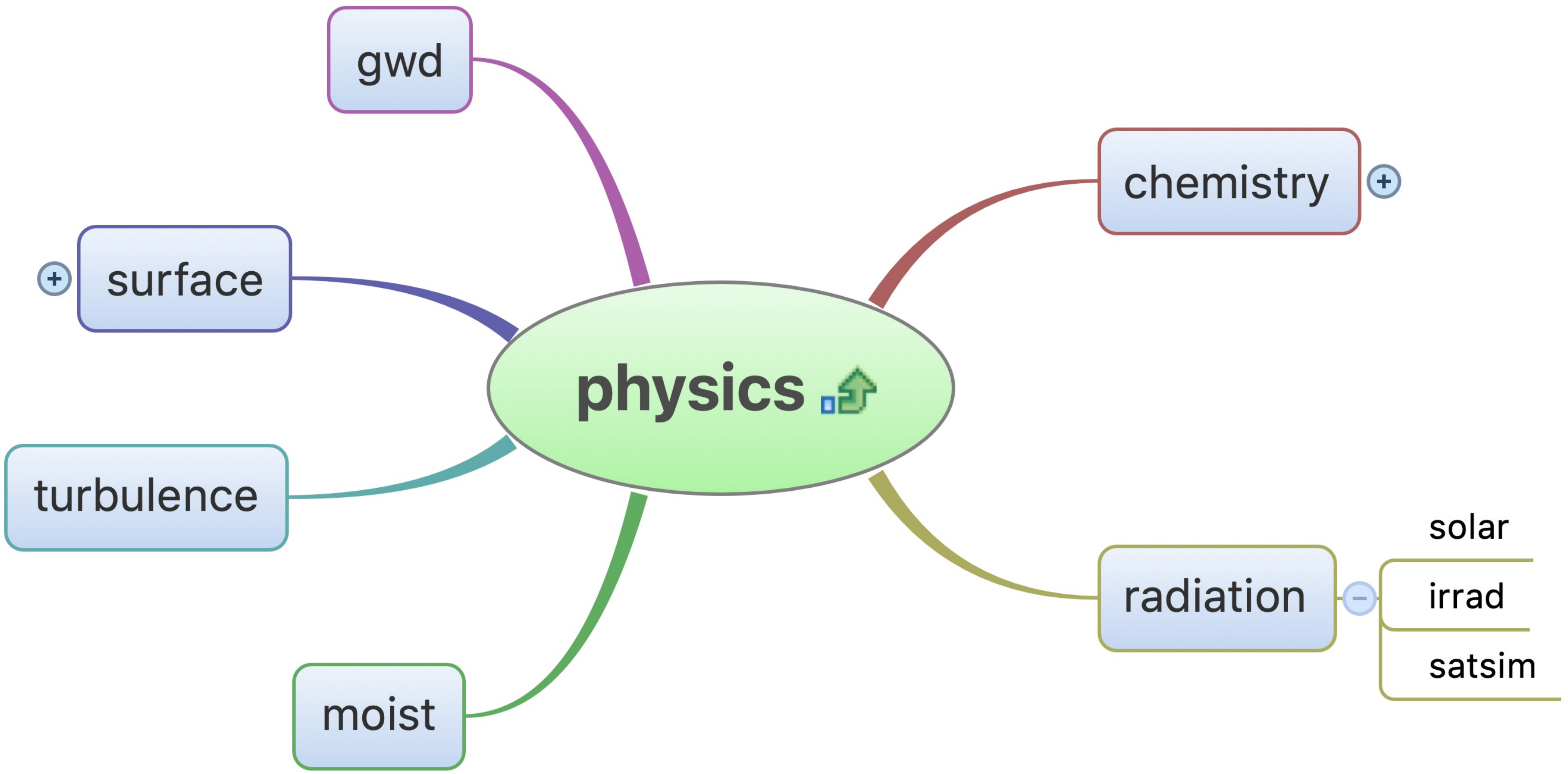


Examples of Physics Interfaces:

How GEOS abstractly interfaces Aerosols to the Model Physics

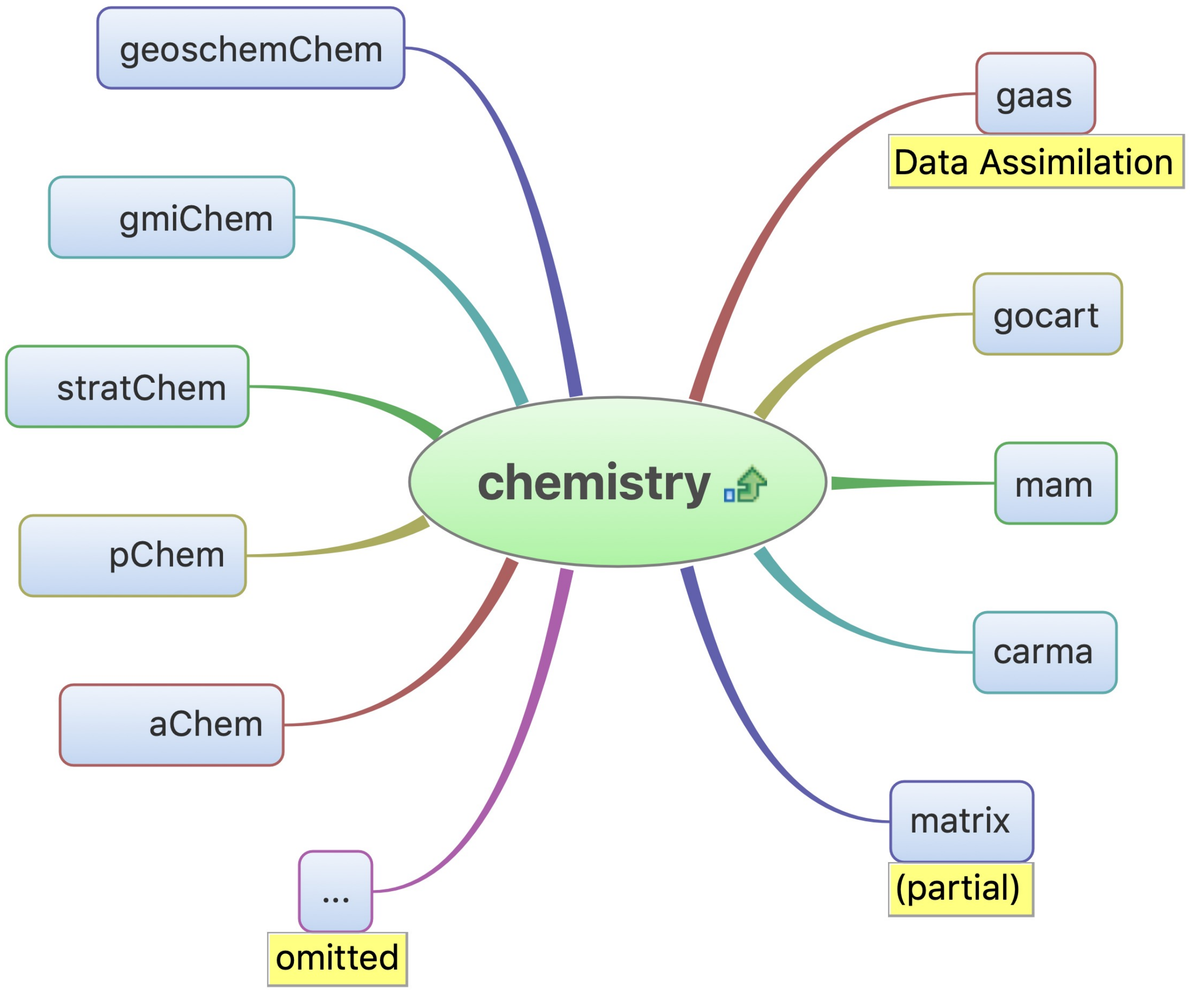
- Radiation
- Cloud Microphysics

GEOS Physics Components



Every entry in this diagram is an ESMF Component

GEOS Chemistry Components



Every entry in this diagram is an ESMF Component

Tight Coupling

- **Aerosol state representation vary widely among different aerosol schemes**
  - **Multiple 3D tracers**
    - Mass concentration
    - Number (modal schemes)
    - Bin sizes (sectional schemes)
  - **Number of tracers:** tens to hundreds
- **With the advent of very high-resolution global chemistry/aerosol models, memory becomes a precious commodity**
  - Exchanging data via tendencies and data copies become prohibitive
  - Example: pre-computation and export of aerosol extinction, single scattering albedo and asymmetry parameter for each band needed by radiation

Encapsulated Coupling via ESMF State Methods

- **Every aerosol component exports, as part of its *Export State*, a single aerosol state**
  - Aerosol State: ***aerosol*** (type: ***ESMF_State***)
  - Each **aerosol** object has several methods attached to it, for example:
    - ***Aerosol_optics***() —— provides extinction, ssa and asymmetry at specific bands
    - ***Activation_properties()*** —— provides properties needed by cloud microphysics, e.g.,

```
real, dimension(:,:,:), pointer :: num            ! number concentration of aerosol particles
real, dimension(:,:,:), pointer :: diameter       ! dry size of aerosol
real, dimension(:,:,:), pointer :: sigma          ! width of aerosol mode
real, dimension(:,:,:), pointer :: density        ! density of aerosol
real, dimension(:,:,:), pointer :: hygroscopicity ! hygroscopicity of aerosol
real, dimension(:,:,:), pointer :: f_dust         ! fraction of dust aerosol
real, dimension(:,:,:), pointer :: f_soot         ! fraction of soot aerosol
real, dimension(:,:,:), pointer :: f_organic      ! fraction of organic aerosol
```

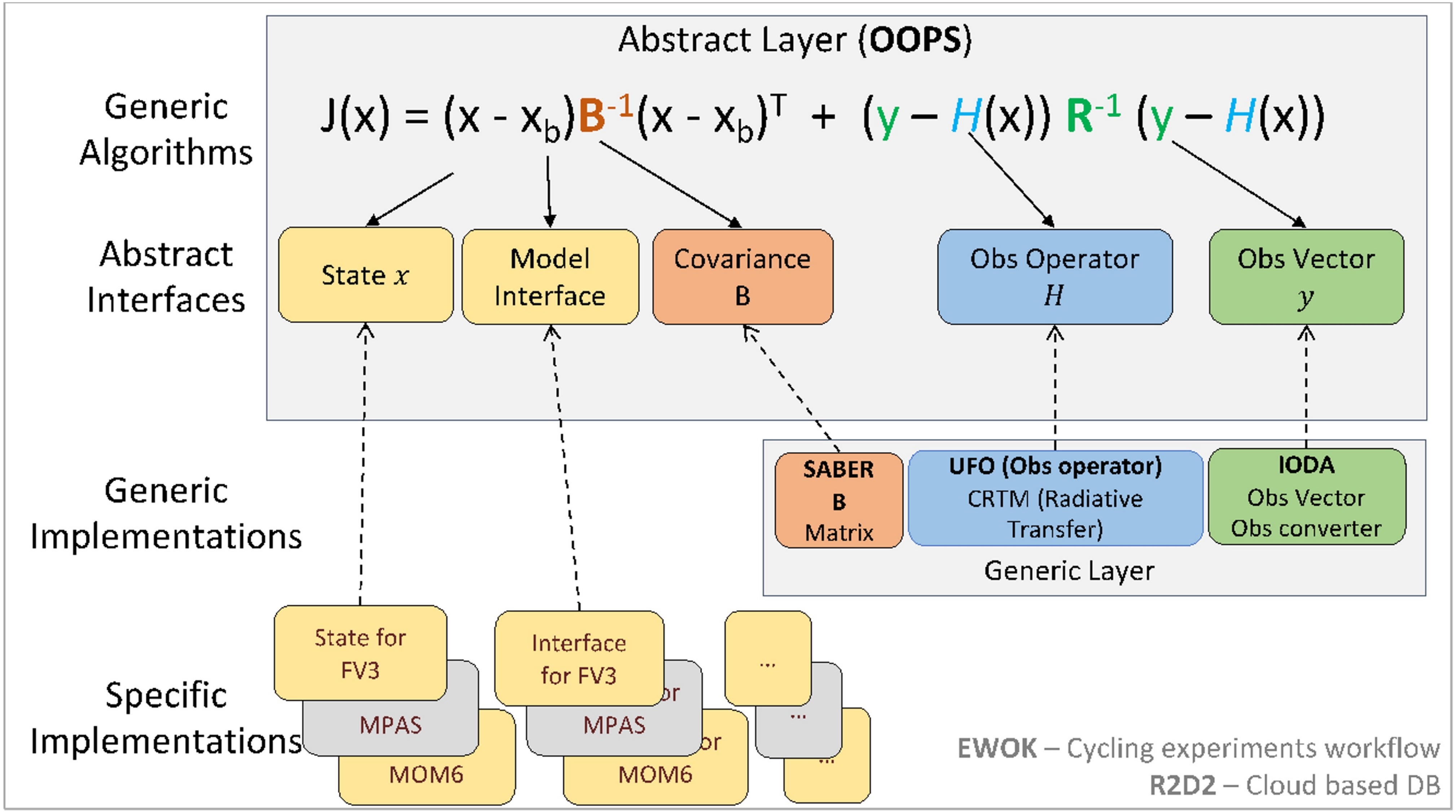
- **Every aerosol component provides this API, whether it implements aerosol microphysics or not, and encapsulates the implementation details inside the state**

Aerosol Data Assimilation

Examples of Aerosol Observables

- **Aerosol Optical Depth (AOD)** is the most commonly available observable
  - Vertically integrated mass weighted by extinction coefficient, summed over multiple species: *low observability*
  - multi-spectral AOD measurements
- **Radiance assimilation**
  - Vector scattering calculations needed for UV-VIS measurements are not cheap
  - Surface BRDF characterization is a challenge
  - Multi-wavelength, multi-angle polarimeter brings much needed information content
- **Surface PM 2.5**
  - Single level
  - Often plagued by representativeness
- **Lidar measurements**
  - Provide vertical profile information
  - Spatially coverage is poor (pencil thin)
  - Attenuated backscatter entangles molecular and particulate scattering with
    - non-linear, non-local obs operator
  - New HSRL concept provides (calibrated) particulate backscatter
    - Linear & local obs operator

JEDI principles:
Build DA blocks once and update for all components of earth-system in one DA system



CRTM Aerosol Schemes

- CRTM version 3.0 continues support aerosol coefficients used in various chemical models and DA systems.
- (Read: CRTM continues to hardwire Aerosol Single Scattering properties for a selection of aerosol schemes. Updates in the aerosol states in these schemes require concurrent changes and PRs to the CRTM repository.)
- The newly added LUTs are the two RTTOV tables based on OPAC and CAMS datasets.
- Users may use any of the following schemes for AOD and aerosol-impacted radiance simulation.
- The primary goal of CRTM team at the current stage is to evaluate the existing aerosol tables, in collaborating with JEDI COMPO and NCAR collogues.

CRTM Version	Model	Aerosol species	Aerosol properties	References
All versions	CRTM (Default)	dust, sea salt, organic carbon, black carbon, sulfate	**effective radius, hygroscopicity (implicit)**	Chin et al., 2002; Han, 2006
v2.4 – v3.0 NetCDF	CMAQ	dust, sea salt, water-soluble, soot, sulfate, water, insoluble, dust-like	effective radius, hygroscopicity (implicit), **radius standard deviation**	Binkowski and Roselle, 2003; Liu and Lu 2016
v2.4.1 – v3.0	GOCART -GEOS5	dust, sea salt, organic carbon, black carbon, sulfate, nitrate (brown carbon is missing)	effective radius, **hygroscopicity**	Colarco et al., 2010
v2.4.1 – v3.0	NAAPS	Bulk aerosol properties: dust, sea salt, smoke, anthropogenic and biogenic fine particles	hygroscopicity	Lynch et al., 2016
v2.4.1 – v3.0	RTTOV-OPAC RTTOV-CAMS	dust, sea salt, organic carbon, black carbon, sulfate, nitrate CAMS: aerosol climatology developed by Copernicus Atmosphere Monitoring Service	effective radius, hygroscopicity	RTTOV v13, https://nwp-saf.eumetsat.int/site/software/rttov/rttov-v13/

Good News: CRTM Generic Interface

In CRTM version 3.1, we will release the **newly developed CRTM generic interface**. As discussed during ICAP 2022, this generic interface will enable optical profiles as input for CRTM AOD and radiance simulations.
This generic interface is independent of the existing CRTM framework and will be of no impact to the existing CRTM users.

The primary optical variables required from users are profiles of optical depth, single-scattering albedo, asymmetry factor, phase function, and directional surface emissivity. For mixture of gaseous, aerosols, and cloud, the input values should be the weighted summary at each layer, for which CRTM will provide an offline Python code for demonstration.

As of October 2023, the forward generic modules are under testing. More development is under planning for the corresponding tangent liner and K-matrix modules.

Questions to ICAP community: is the forward calculation sufficient? **Will you also request the TL and K-matrix modules?**

If you are interested in discussing more about this interface or CRTM in general, please send me an email.
If you are going to AGU 2023 Fall Meeting, let's catch up in San Francisco! Cheng Dang, dangch@ucar.edu

Community Exercise

Practicing Interoperability within the ICAP Community

Results to be presented during ICAP 2024

Aerosol Single Scattering Properties

- Premise: every aerosol modeler knows to compute some of these from their representation of *Aerosol State*
  - Extinction profiles (and by extension AOD)
  - Single scattering albedo profiles
  - Asymmetry parameter, phase function or full phase matrix
  - Wavelengths: from the UV to the TIR
- Note:
  - Although a generic interface to a community-maintained Mie/T-matrix codes could be extremely useful for controlled model intercomparisons (say, ensuring consistent fundamental assumptions) …
    - Pete has one (wink, wink)
  - … consistency with the ESM in which the aerosol component exists will always be needed.

Possible Goals of such a Project

- Simple python implementation of *Aerosol States* subclassing from a generic class for key ICAP models
  - GEOS
  - NAAPS
  - CAMS
  - Who else?
- Develop Surface Models (file based)
  - Hyperspectral BRDF
  - Emissivity
- Develop observation operators for key observables
  - Multispectral AOD (UV to TIR)
  - Multispectral profiles of extinction, SSA and g
  - Reflectances from UV to SWIR (say, VIIRS)
  - Brightness temperature for the TIR with aerosol effect.
- At least a couple of RT backends

Possible Radiative Transfer Backends

- VLIDORT
- GRASP RT model (Lille 6s heritage)
- CRTM
- RTTOVS

Phase I Experiment

- Instantiate *Aerosol State* for a set of golden dates, given files from your system
- Provide surface representation
- Could ignore clouds and gas corrections to begin with
- Simulate and intercompare key observables
  - Simulators work with abstract *Aerosol State* and surface
- Test sensitivity on backend RT codes: UV, VIS, TIR
- Development environment:
  - GitHub repo with GitHub flow
  - All software must be open source to participate
  - Platform: NASA/AWS Science Managed Cloud Environment (SMCE) – TBD. This would enable international participation (with some restrictions).

Next steps

- Form a small group of interested participating individuals
  - Write to arlindo.m.dasilva@nasa.gov if interested
- Meet and come up with:
  - Clear project objectives and expected outcome
  - Project plan with milestones and schedule
- Establish recurring meetings
- BYOF: bring your own funding