



PACE for Earth System Modeling

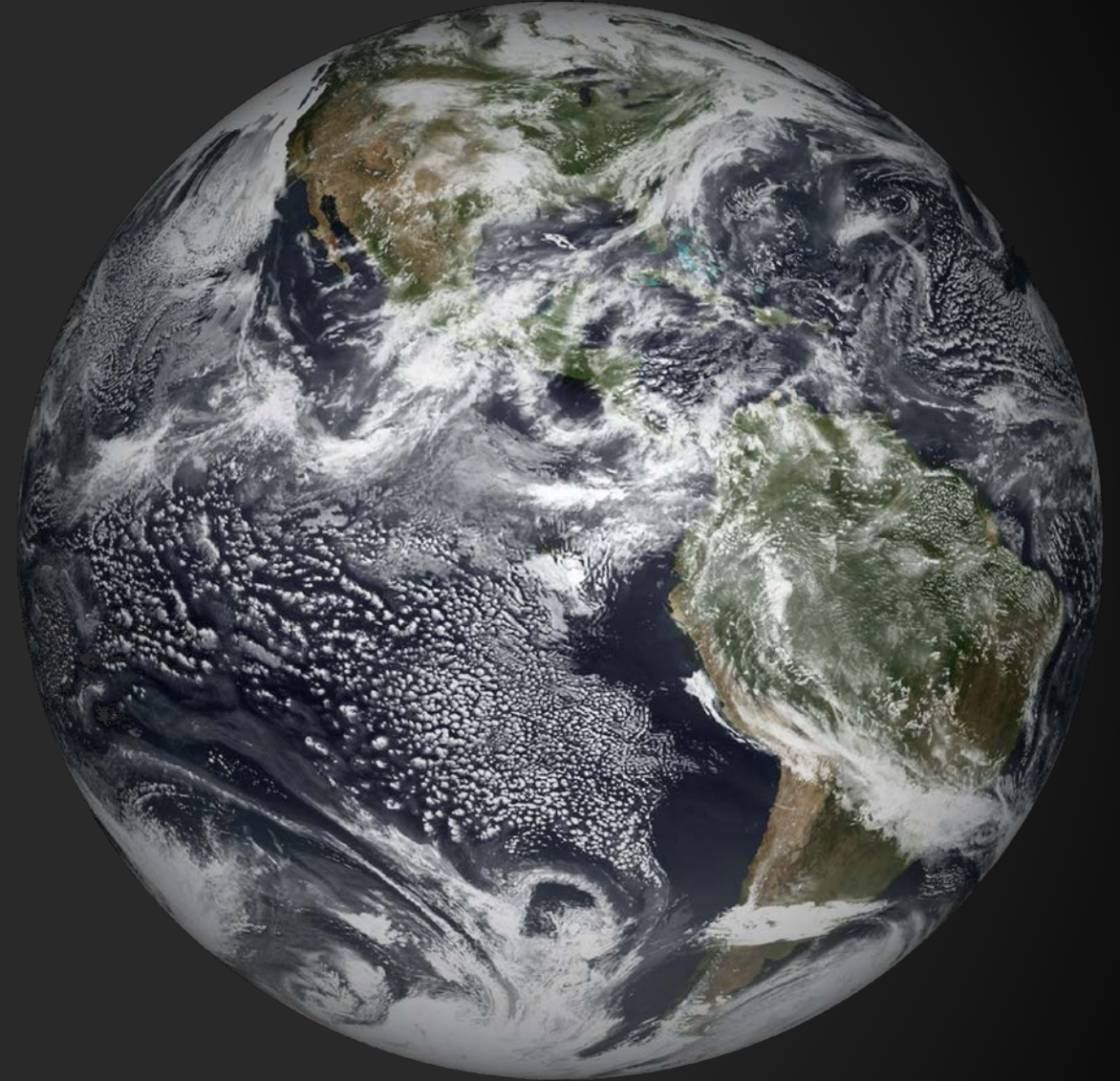
Arlindo da Silva, P. Castellanos, W. Putman, A. Molod, C. Keller, E. Knowland
L. Ott, C. Rousseaux

*Global Modeling and Assimilation Office
NASA/Godard Space Flight Center*

PACE Class
University of Maryland Baltimore County (and GSFC)
1-5 Aug 2022

Outline

- Overview of Earth System Models (ESMs)
- Using ESMs for PACE Observing System Simulation Experiments (OSSEs)
- Main Components of Earth System Models and potential **PACE contributions**
- Concluding Remarks

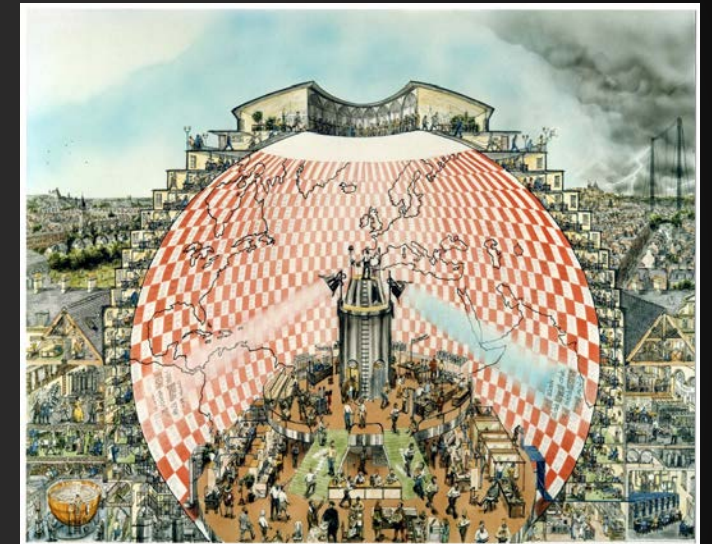


Atmospheric Models in ~10 Years

- Cloud/storm resolving models
 - Regional models (short range) → sub km to 1 km
 - Global forecast models (extended range up to 10 days) → ~1-5 km
- Aerosol models
 - Regional models (short range) → sub km to 4 km
 - Global forecast models (ext. range) → ~3-5 km
- Climate models: (long-term, years) → 25 km
- Unified Models: scalable from CRM to Regional to Climate
- More coupling
 - New components: composition, land, applications (fire/urban)
- Advances in Model Physics
 - New methods (Lagrangian, Bayesian), increased complexity
- Advances in data assimilation/evaluation
- **Processes more important as scales collapse**

ACCP Modeling Workshop Workshop (BAMS 2021)

BAMS Report

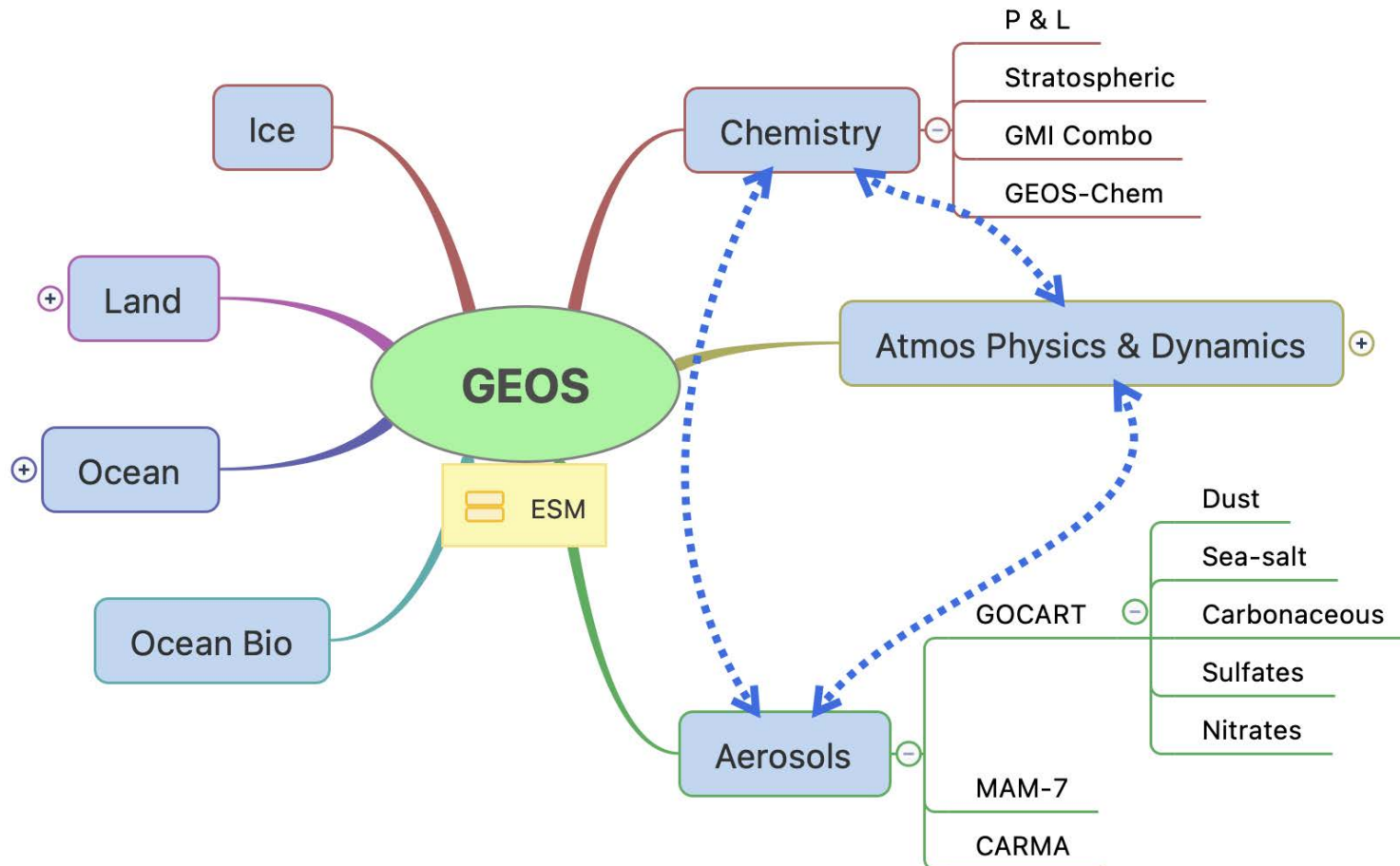


"Perhaps some day in the dim future it will be possible to advance the computations faster than the weather advances... but that is a dream."

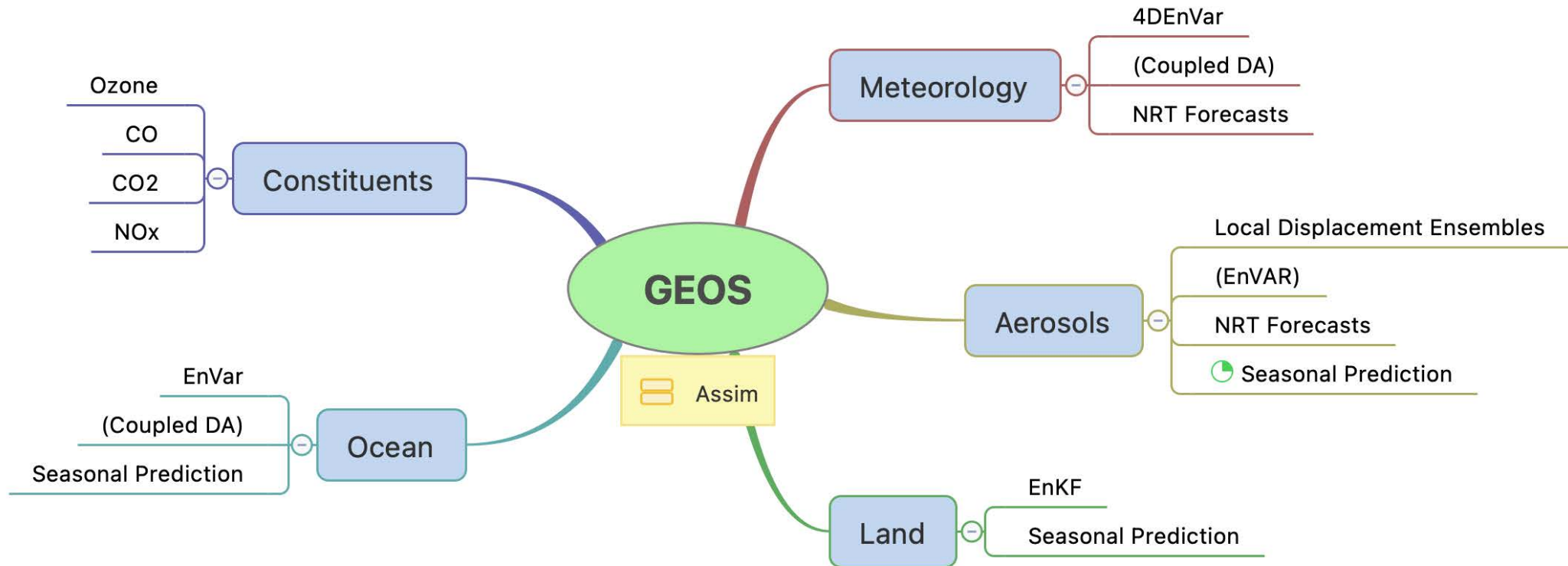
L. F. Richardson



GEOS Earth System Model



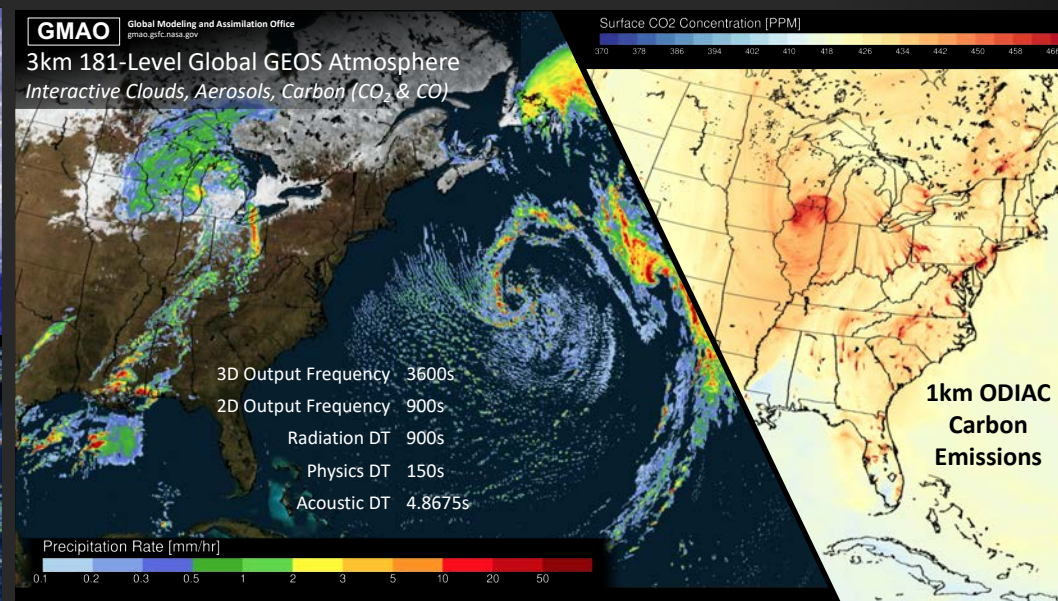
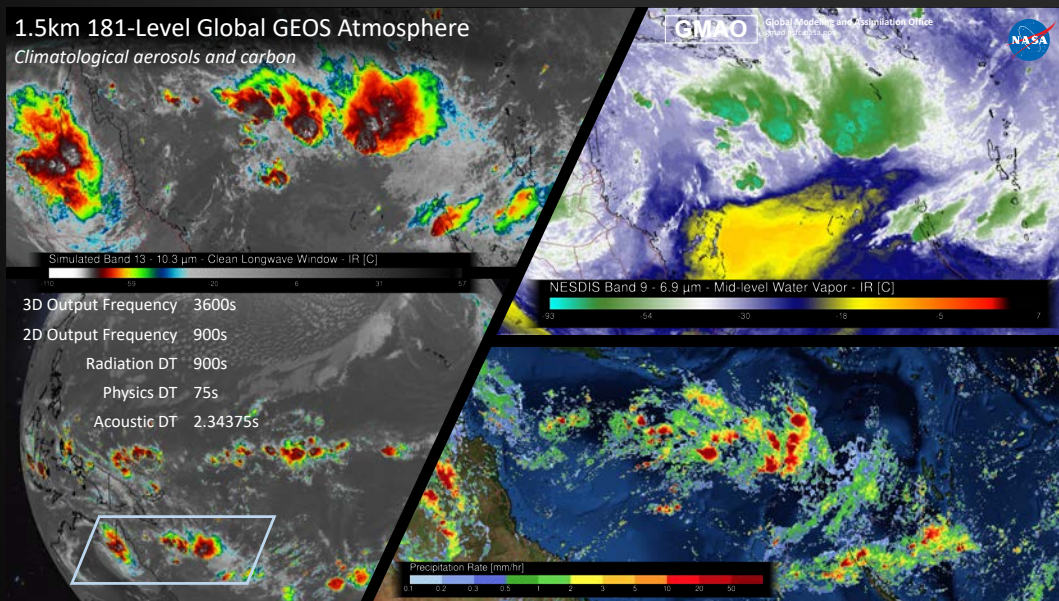
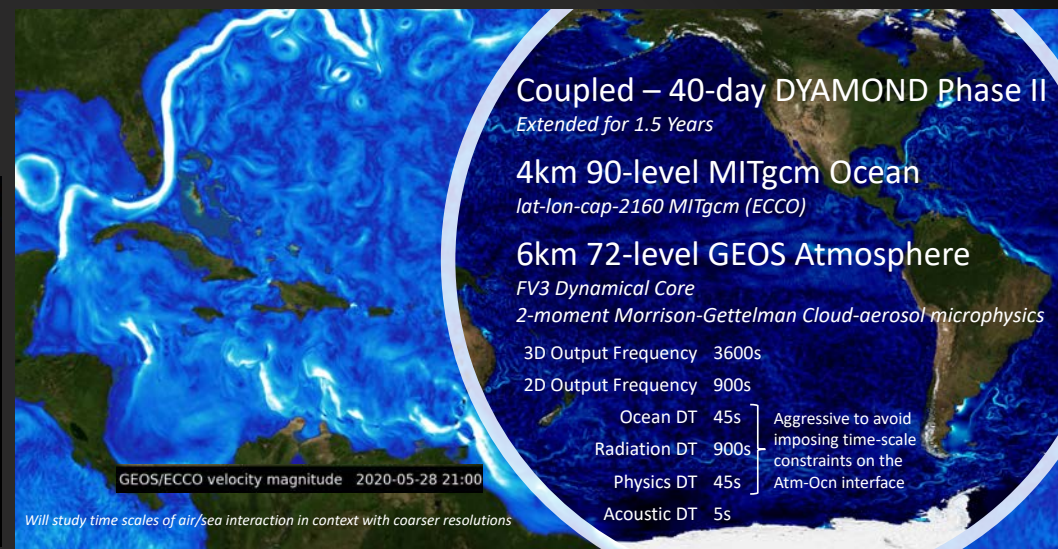
GEOS Data Assimilation



Systems migrating to the JEDI Framework

Global Storm Resolving Simulations

| Configuration | Total Cores - "System" | Throughput | Data Volume |
|--|--|---------------------------------------|---------------|
| Coupled Atm-Ocn 6km 72-Level Atm 4km 90-Level Ocn | 8,160 Intel Xeon Haswell processor cores "Pleiades" NASA-NAS | 3 Simulated Days / Wallclock Day | 0.3 Petabytes |
| Atmosphere+Aerosols 3km 181-Level Atm | 39,360 Intel Xeon Skylake processor cores "Discover" NASA-NCCS | 7 Simulated Days / Wallclock Day | 2.0 Petabytes |
| Atmosphere 1.5km 181-Level Atm | 39,440 Intel Xeon Skylake processor cores "Discover" NASA-NCCS | 1.5 Simulated Days / Wallclock Day | 1.3 Petabytes |

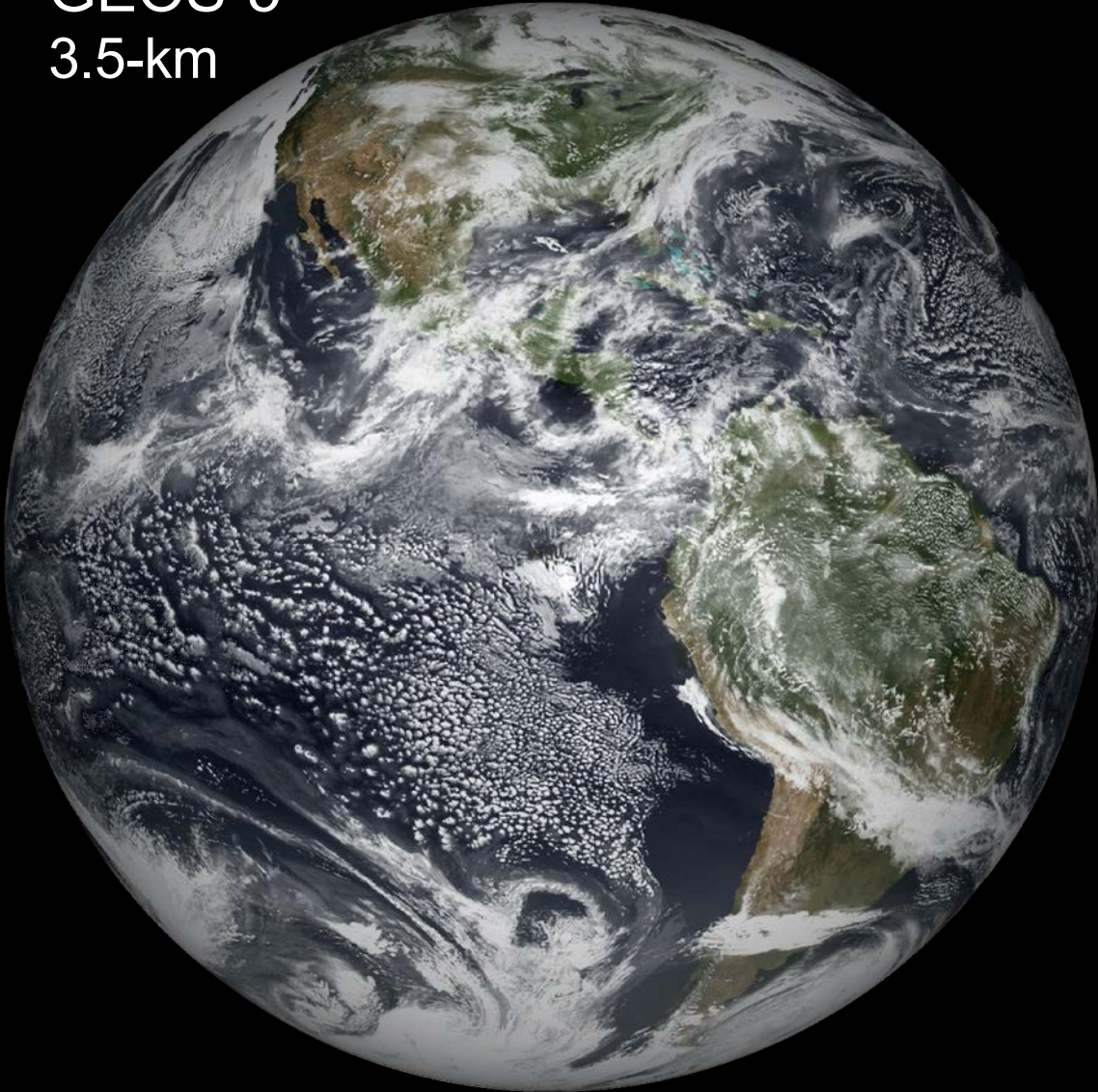


Model resolution \approx Satellite scales

~50-million pixels

GEOS-5

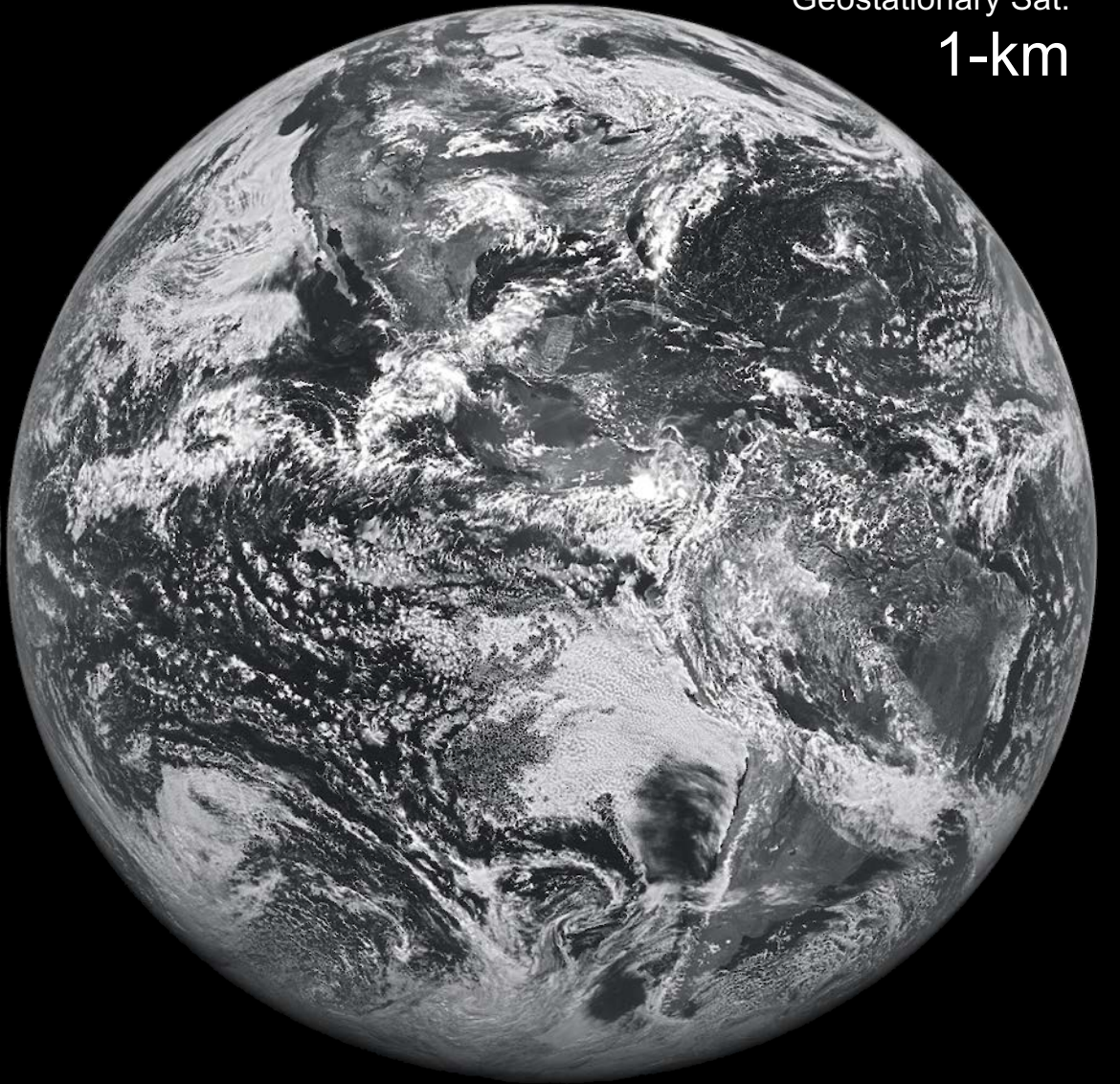
3.5-km



~200-million pixels

Geostationary Sat.

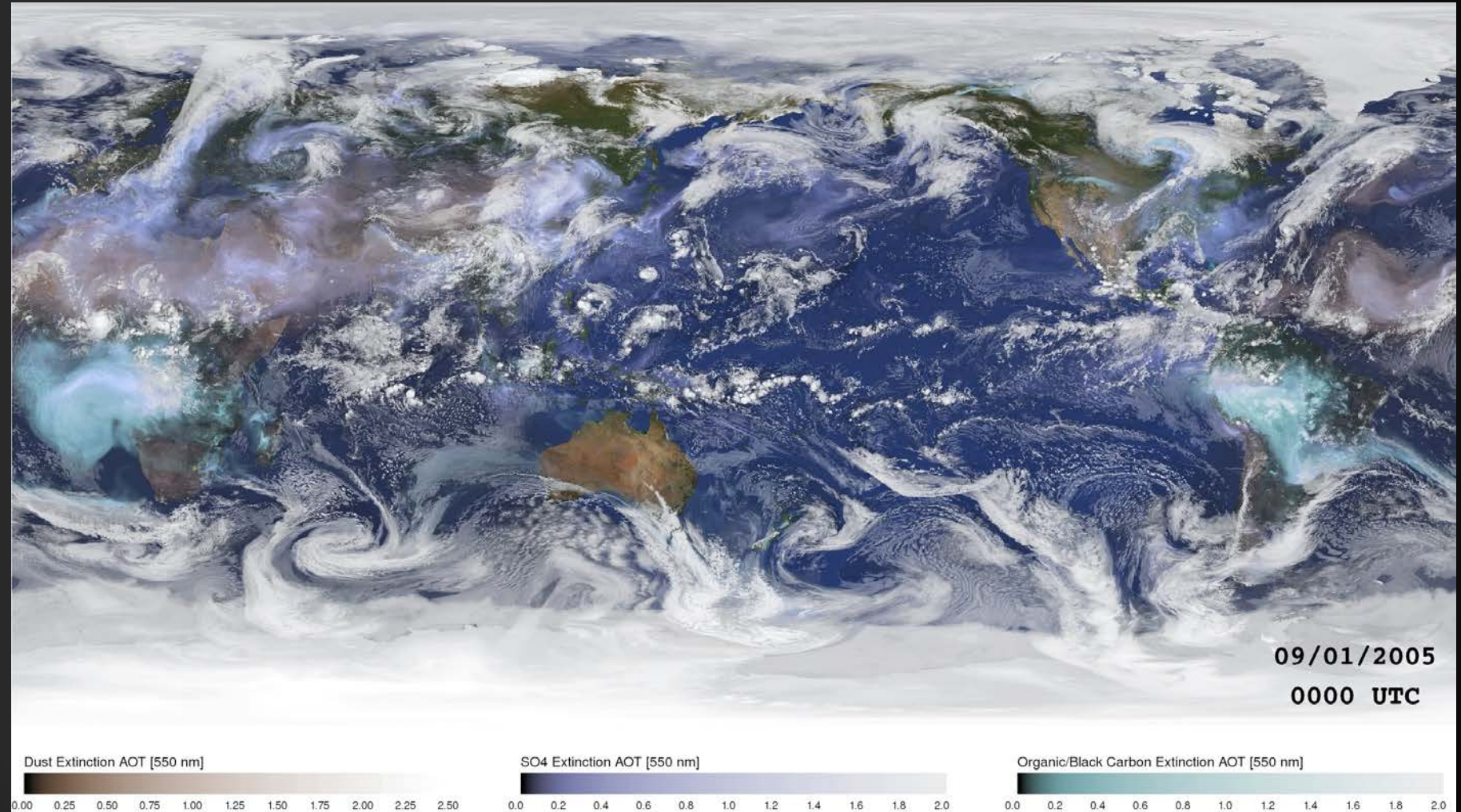
1-km



Global 7km GEOS Nature Run

Clouds

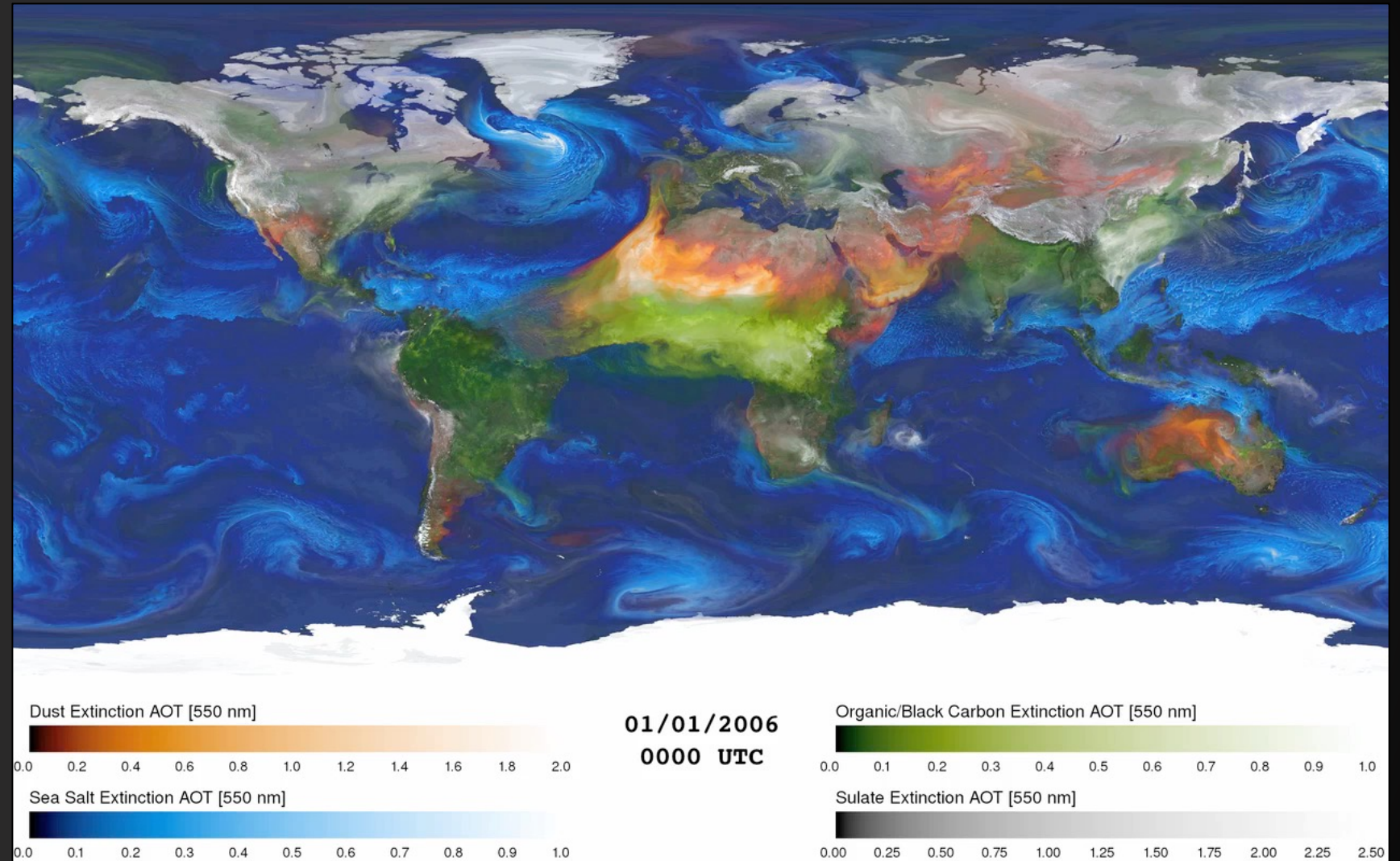
Clouds have a critical role in the Earth's weather/climate system. With horizontal resolution increased to 7-km, GEOS-5 now becomes capable of resolving clusters of clouds rather than simply relying on the statistical effects of clouds over large grid boxes. Cloud systems of the ITCZ, tropical storms, and mid-latitude storms begin to resemble clouds as observed from space.



Global 7km GEOS Nature Run

Global Aerosols

Aerosols play an important role in both weather and climate. They are transported around the globe far from their source regions, interacting with weather systems, scattering and absorbing solar and terrestrial radiation, and modifying cloud micro- and macro-physical properties. They are recognized as one of the most important forcing agents in the climate system.

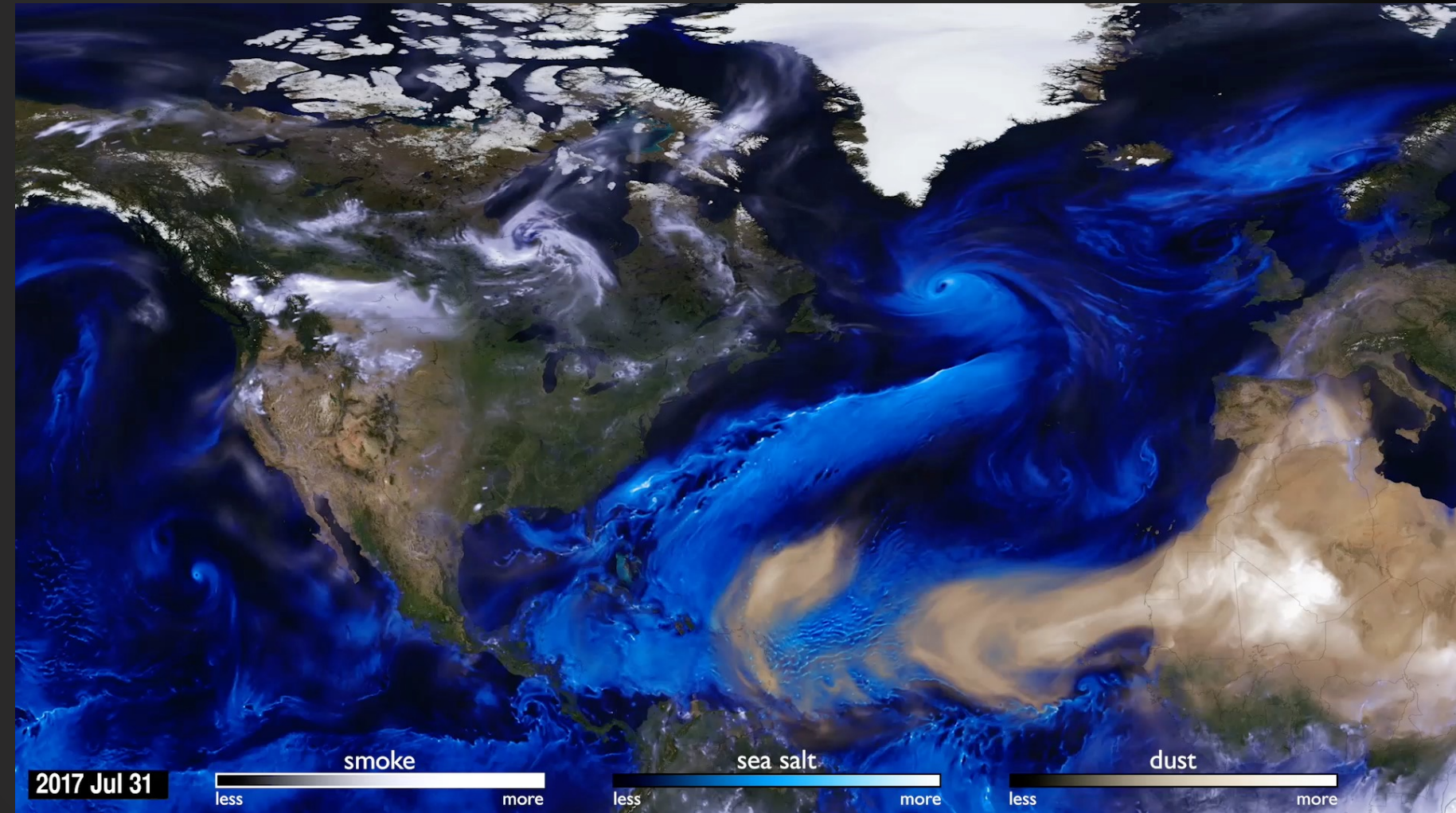


GEOS Model – 2017 Hurricane Season

Hurricanes and Aerosols

Hurricanes and tropical storms are depicted by the large concentrations of sea salt particles caught up in their swirling winds. The dust blowing off the Sahara, however, gets caught by water droplets and is rained out of the storm system, and aerosol radiative effects can contribute to storm invigoration.

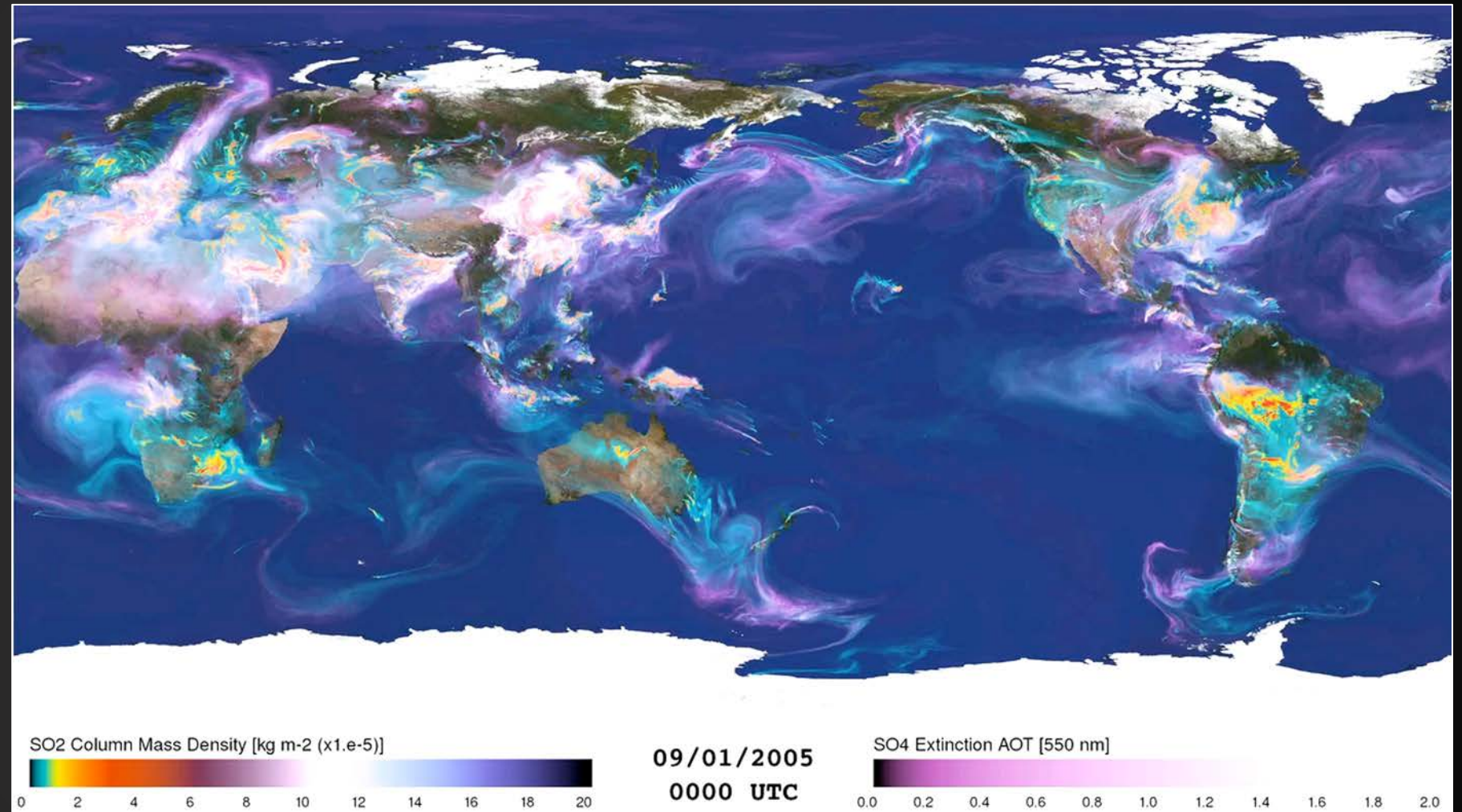
Smoke from the massive fires in the Pacific Northwest region of North America are blown across the Atlantic to the UK and Europe. This visualization is a result of combining NASA satellite data with sophisticated mathematical models that describe the underlying physical processes.



Global 7km GEOS Nature Run

Sulfur Dioxide Sulfate Aerosols

Sulfur dioxide (SO_2), produced during the burning of fossil fuels and from volcanic eruptions, is a short lived gas which can act as pollutant near the surface with detrimental health and acidifying effects. With a mean life time of just a couple of days in the troposphere, emitted SO_2 is quickly converted to sulfate aerosol (SO_4) through oxidation by OH or by reaction with H_2O_2 within clouds. The resulting SO_4 exerts a direct radiative effect on the atmosphere and it can also have an indirect radiative effect by inducing changes in cloud and precipitation microphysics.



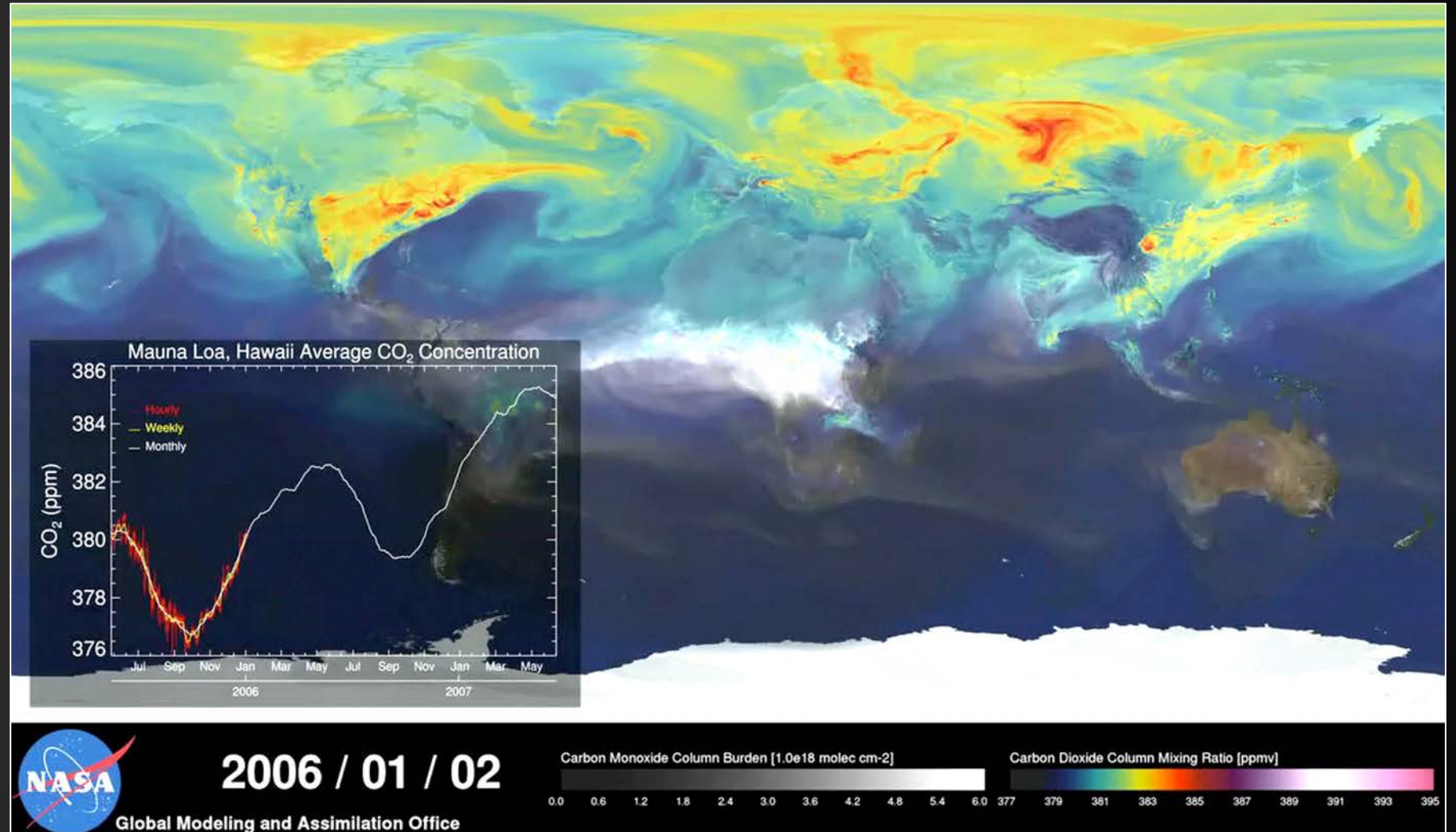
Global 7km GEOS Nature Run

Carbon Dioxide

This visualization shows column concentrations of atmospheric CO₂ (colored shades) and CO (white shades underneath) from January 1, 2006 to December 31, 2006.

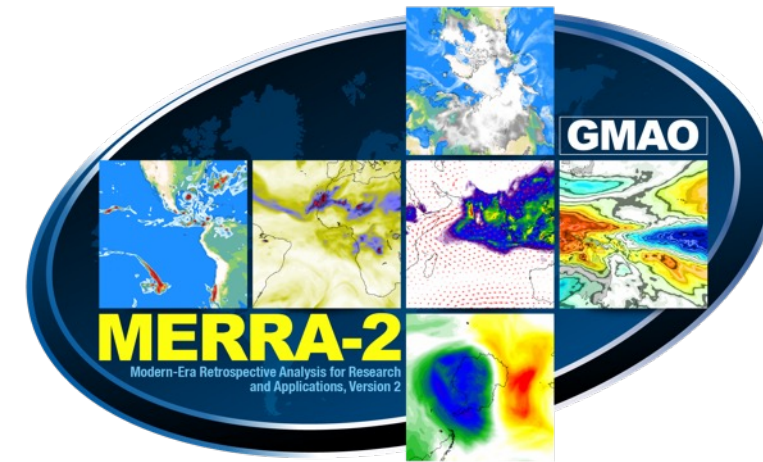
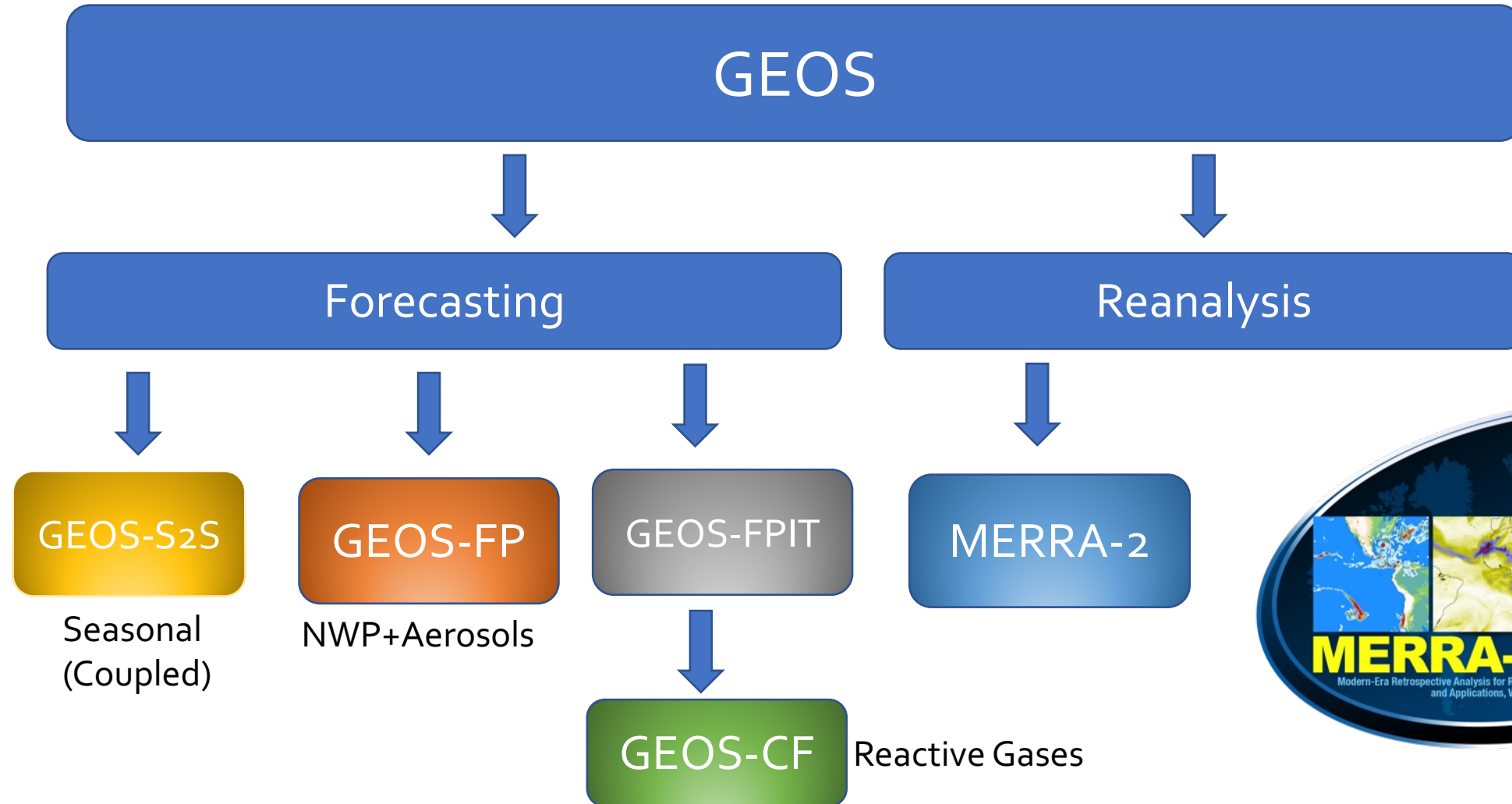
CO₂ variations are largely controlled by fossil fuel emissions and seasonal fluxes of carbon between the atmosphere and land biosphere. CO₂ concentrations are enhanced by carbon sources, mainly from human activities. During Northern Hemisphere spring and summer months, plants absorb a substantial amount of CO₂ through photosynthesis, thus removing CO₂ from the atmosphere.

Atmospheric CO, a pollutant harmful to human health, is produced mainly from fossil fuel combustion and biomass burning. Here, high concentrations of CO (white) are mainly from fire activity in Africa, South America, and Australia.



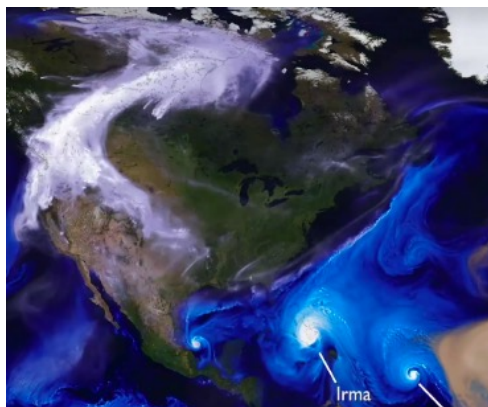
GMAP Global Products

National Aeronautics and
Space Administration

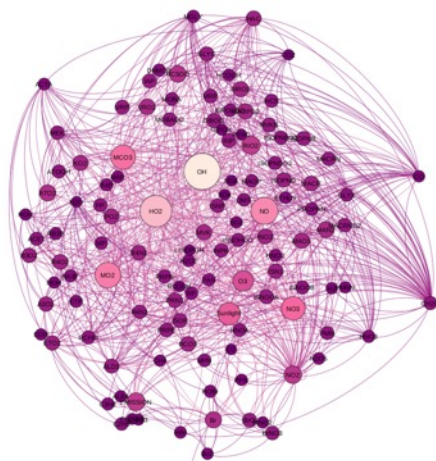


GEOS Composition Forecast (GEOS-CF)

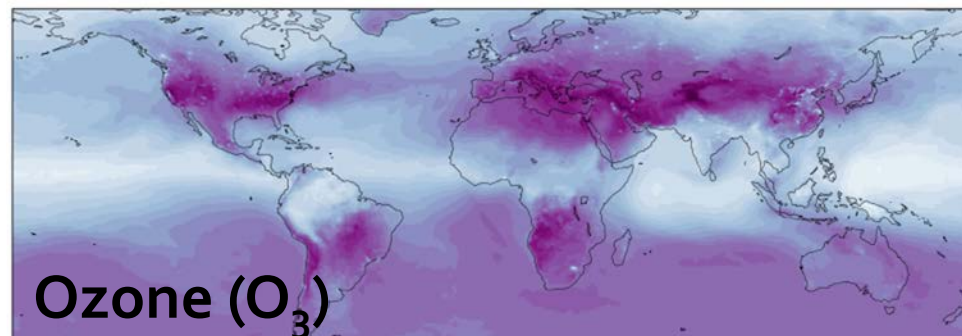
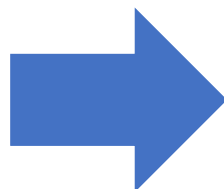
National Aeronautics and
Space Administration



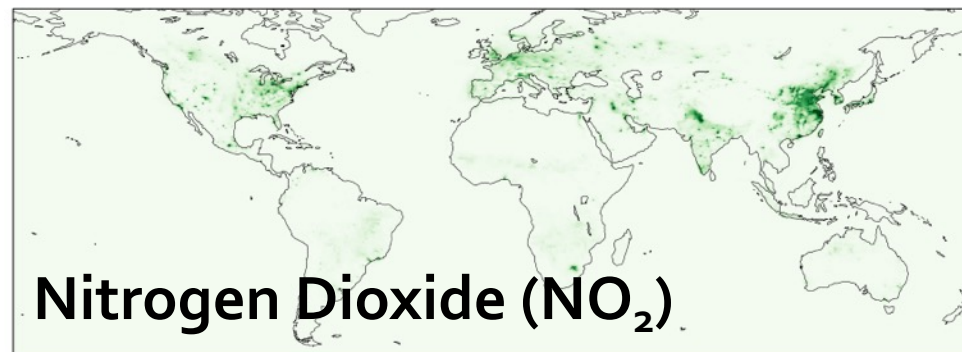
GEOS NWP



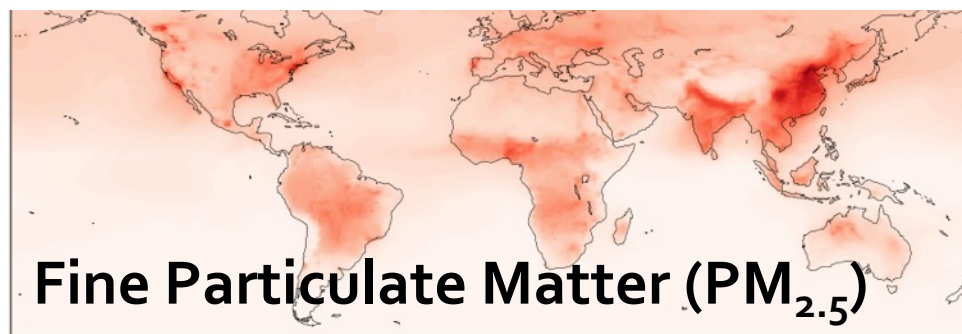
GEOS - Chem



Ozone (O_3)



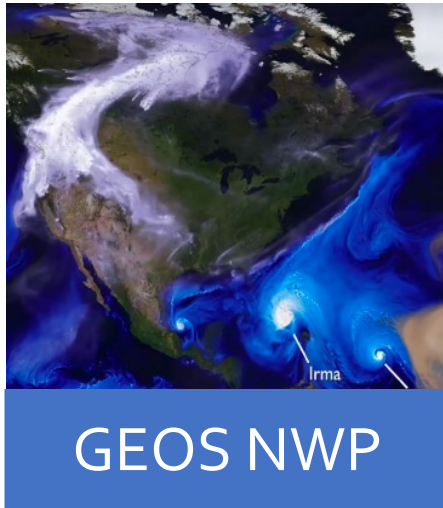
Nitrogen Dioxide (NO_2)



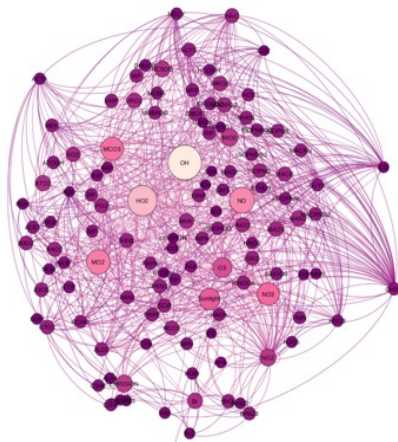
Fine Particulate Matter ($PM_{2.5}$)

Chemical Data Assimilation System for Reactive Gases

National Aeronautics and
Space Administration



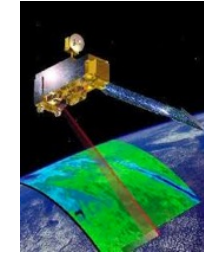
GEOS NWP



GEOS - Chem

Data Assimilation
System
 CO , NO_x , O_3

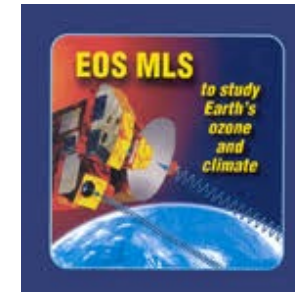
Weakly coupled; 6 hour
assimilation window



MOPITT



OMI



MLS

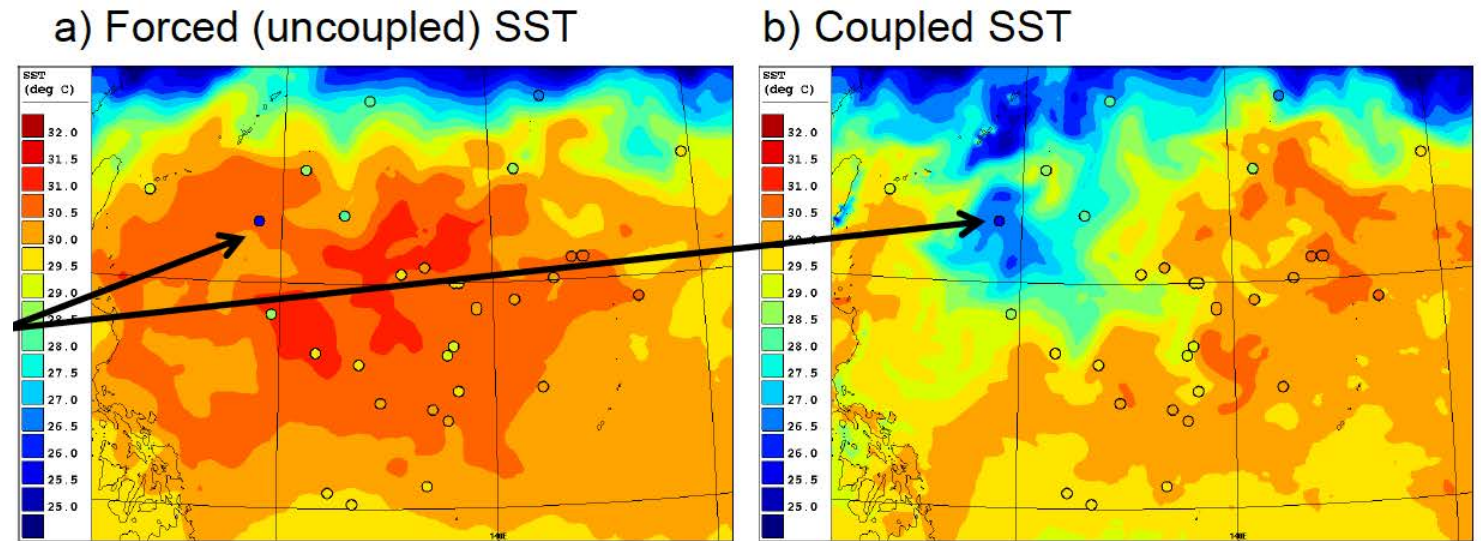


PACE

NO_2 , O_3 ?

Benefits of Air-sea Coupling for NWP

Much better
agreement with drifter
buoys of the SST in the
cold wake behind
Typhoon Neoguri



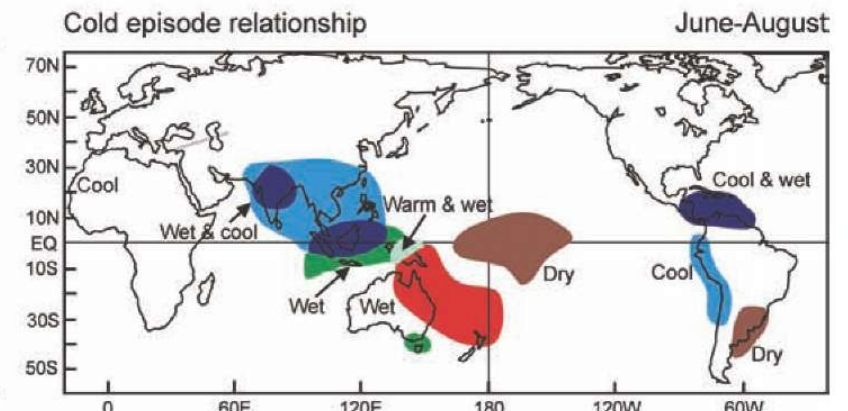
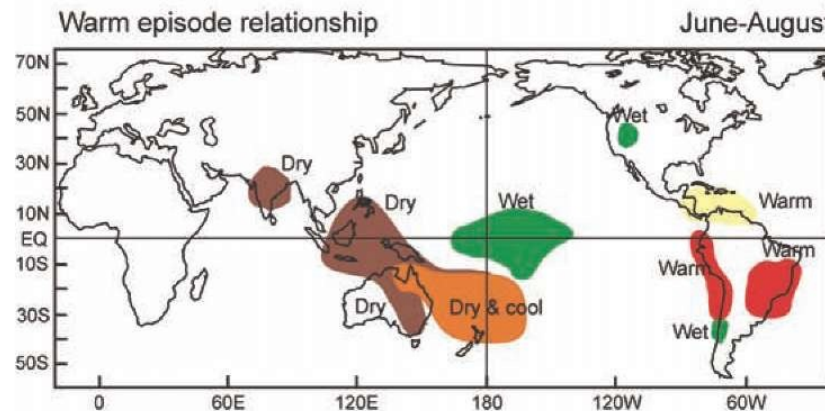
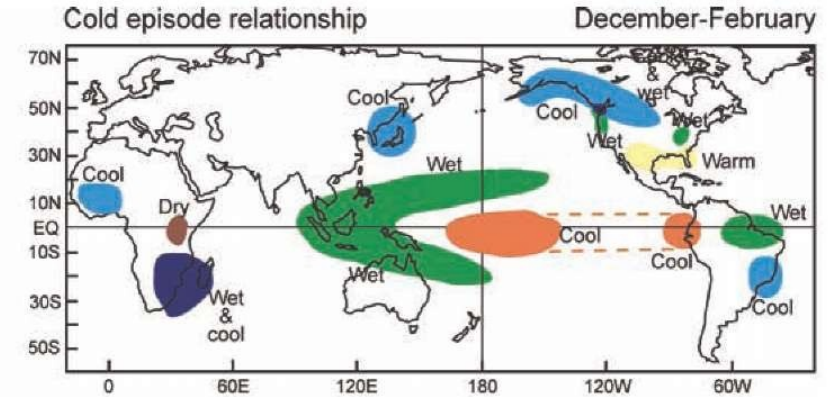
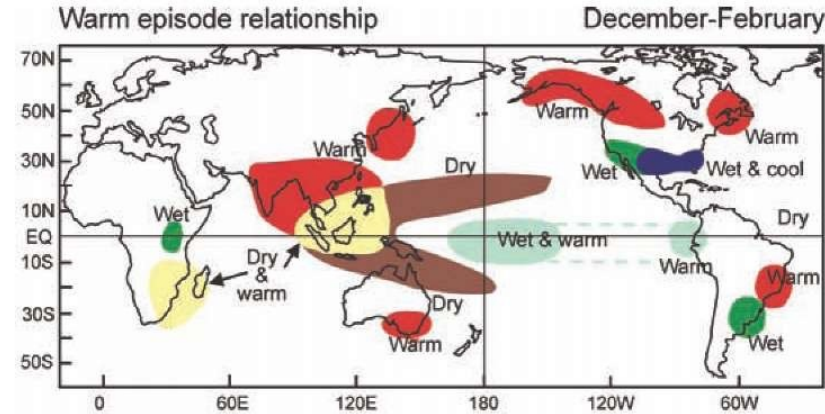
Smith et al., 2018, MWR

Knowledge of the vertical stratification of the ocean is crucial to being able to predict the coupled feedback and thereby predict the evolution of tropical cyclones.

Seasonal Prediction

ENSO is the biggest driver of seasonal prediction and predictability, but other modes of variability contribute as well, *i.e.*, NAO, PNA, IOD.

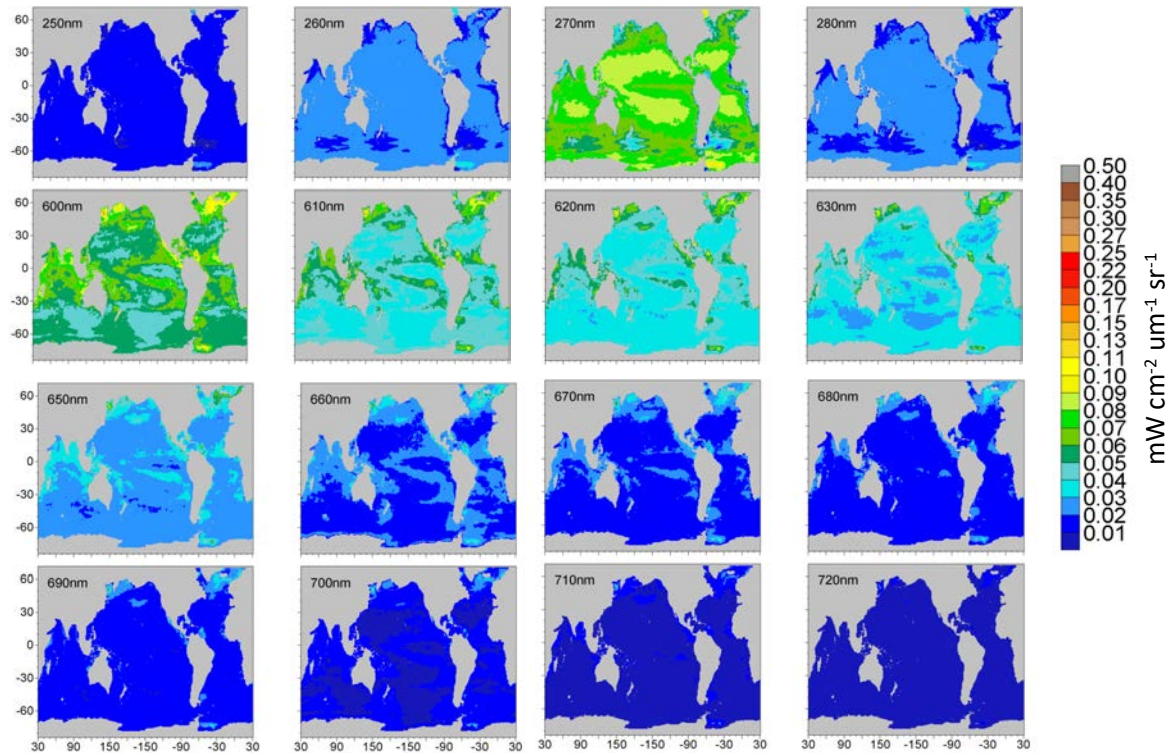
Atlantic SST is important too, gradients of SST (Atlantic dipole) can impact the location of the Atlantic ITCZ. The Atlantic Meridional Mode is also a strong mode of variability there.



Extratropical predictability is mostly based on ENSO (and other mode) teleconnection patterns.

PACE and ocean biogeochemical modeling:

Using the NASA Ocean Biogeochemical Modeling in preparation for PACE



Model normalized *water-leaving radiances* for selected wavelengths in the ultraviolet, long visible, and near-infrared region.

Rousseaux, C.S. (PI) "Phytoplankton Composition algorithms for PACE".

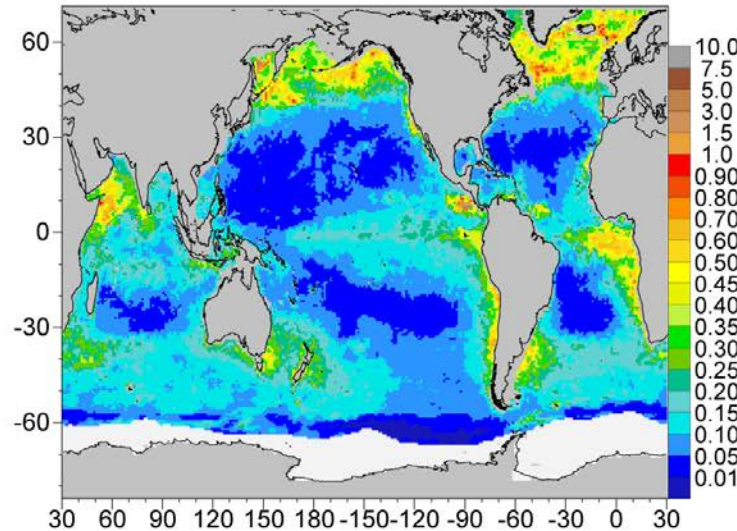
PACE Science Team (NNH13ZDA001N-PACEST), Grant # NNX15AE81G, 2015-2019;

- Produced a 1-nm simulated upwelling radiance data set using the **NOBM** and the Ocean-Atmosphere Spectral Irradiance Model (**OASIM**)
- This simulated dataset was validated against existing multispectral ocean color satellite data
- The simulated dataset was used in several applications. For example:
 - Test the effects that spectral and directional light have in simulations of ocean radiative transfer model ([Gregg and Rousseaux 2016](#)).
 - Develop a test granule simulation to use for algorithm development and other post-processing efforts by the PACE Project Team (GMAO and PACE Project collaboration-POC: Patricia Castellanos).

PACE and Ocean Biogeochemical Modeling: Using ocean biogeochemical models after launch

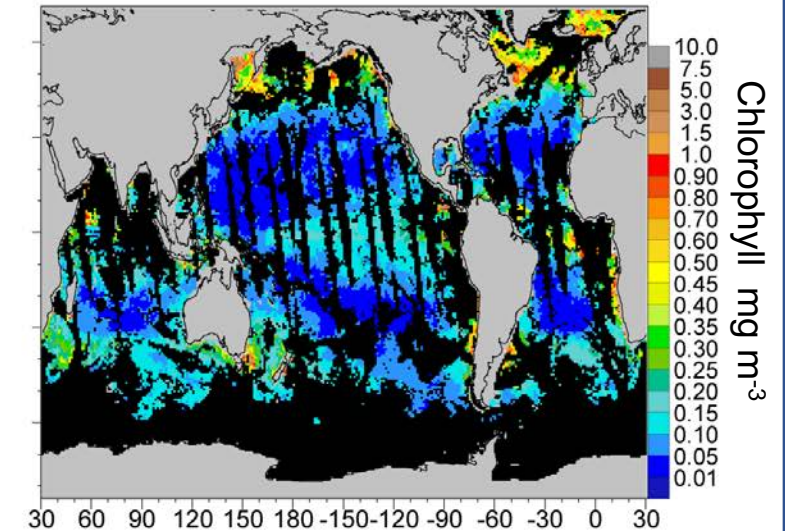
- The new era of hyperspectral data will open the door to a series of applications and challenges. Biogeochemical models provide a platform to integrate/assimilate the increasing number of data (whether in resolution or variables available)
- The **assimilation of satellite ocean color** provides global coverage (some regions such as the Southern Ocean can lack satellite data for >6 month of the year) as well as products for which algorithm do not currently exist (e.g., nutrients, phytoplankton groups, etc)
- Biogeochemical models also provides a **platform to integrate datasets** (parametrize, assimilate and forcing), conduct sensitivity analysis (e.g., algorithm development, instrument design) and provide data in an earth system framework (e.g., climate monitoring, carbon projections etc.)

Assimilated VIIRS Chlorophyll Sep 1 2013



Ice fields are shown in white.

Daily VIIRS Chlorophyll Sep 1 2013



Missing data is shown in black.



OSSEs

Detailed Simulation of PACE Measurements before Launch



O.S.S.E

Observing System

Simulation

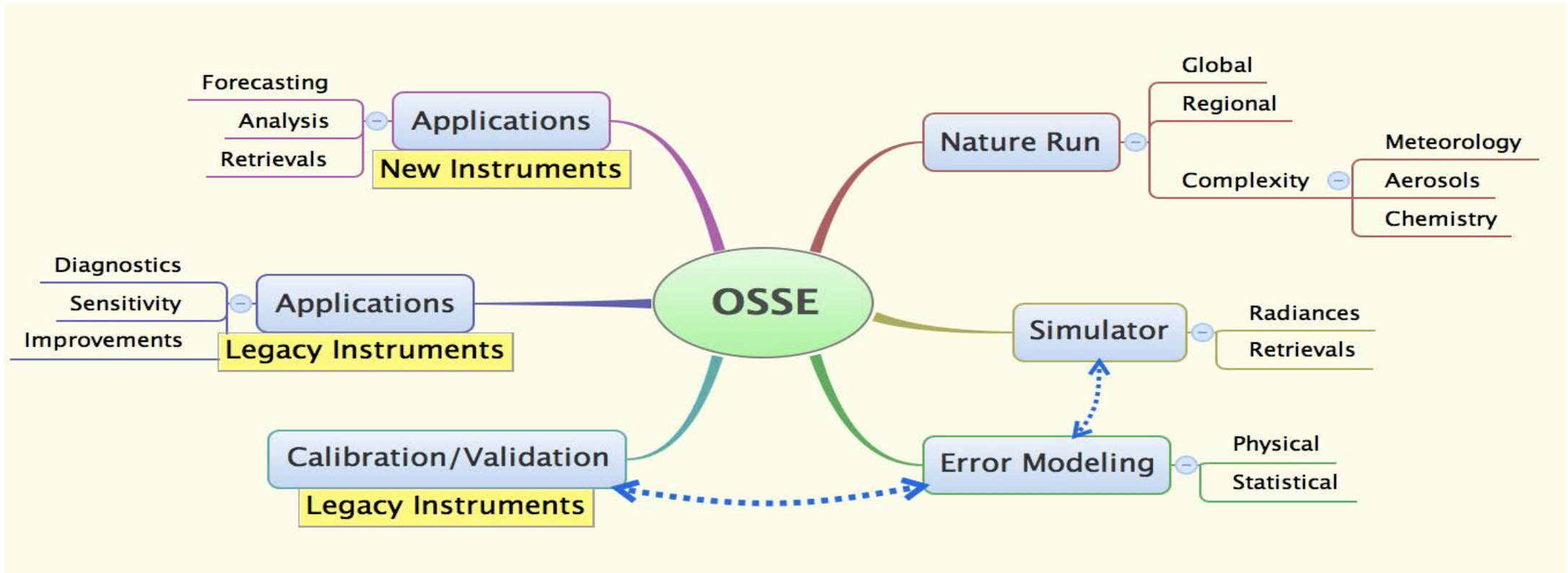
Experiment

Model-based OSSE

A framework for numerical experimentation in which *observables* are simulated from fields generated by an earth system model, including a *parameterized* description of the *observational error* characteristics.

Simulations are performed in support of an experimental goal.

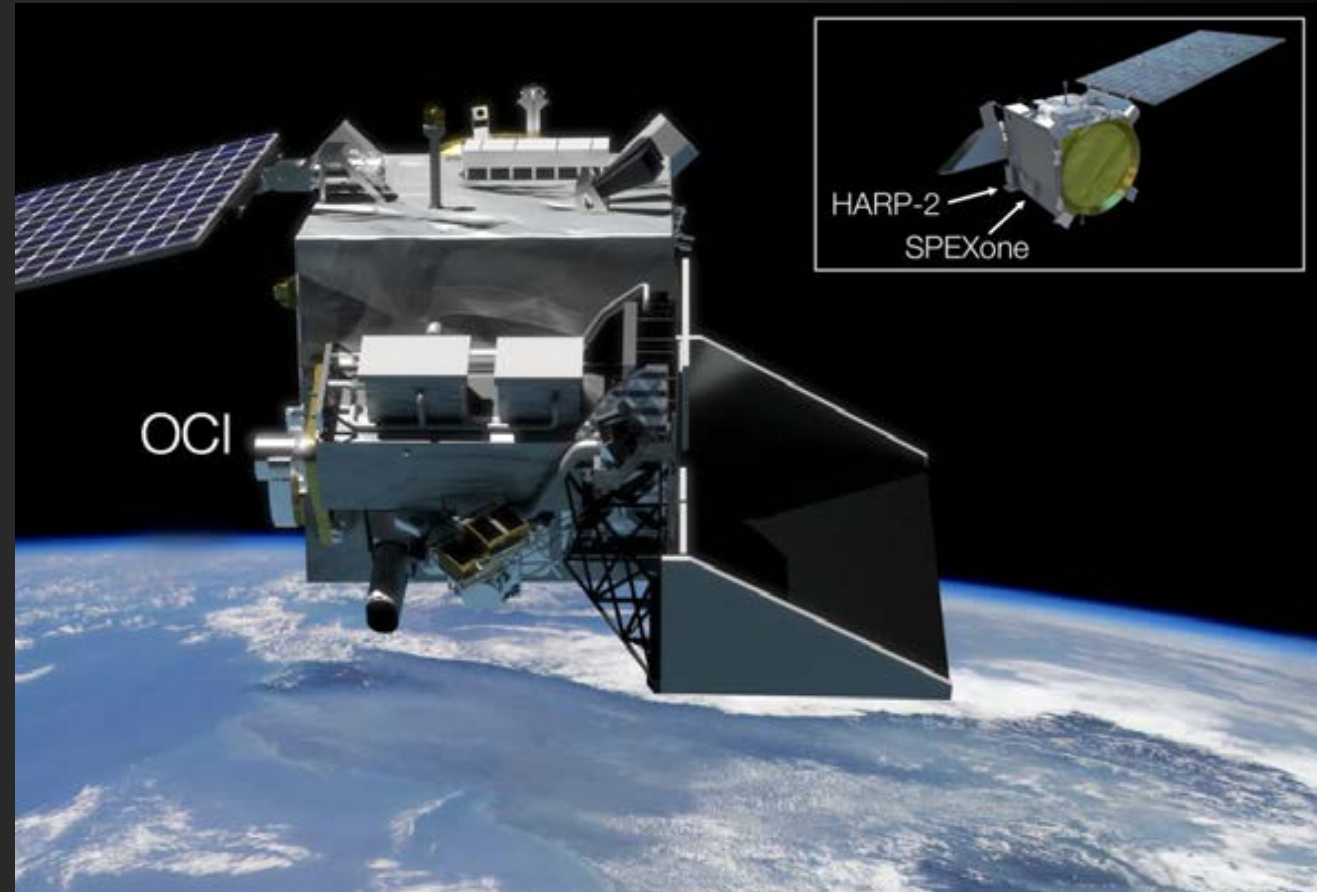
Elements of an OSSE System



As with any simulation, OSSE results apply to new instruments only to the degree they have been validated with existing legacy instruments.

Simulation of PACE Measurements for Ocean Color and Aerosol Retrievals

1. Earth System Model
Components of relevance
 - Ocean biogeochemistry
 - Atmospheric aerosols
 - Trace gases
2. Ocean surface radiance simulation
3. Top-of-atmosphere radiance simulation

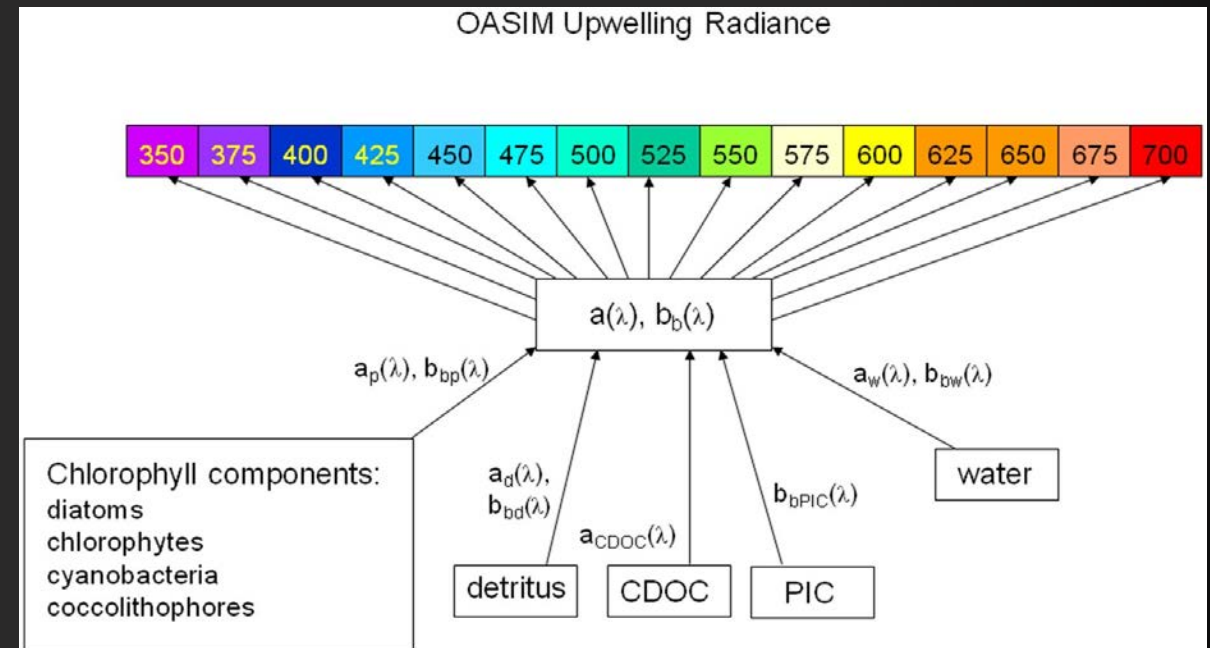
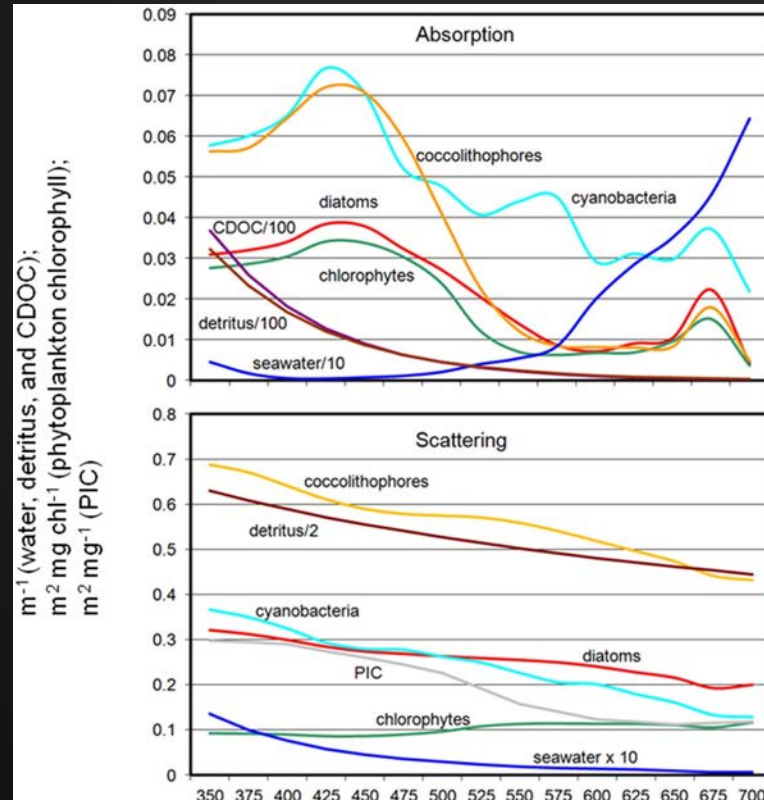


Global Ocean Radiance Simulation

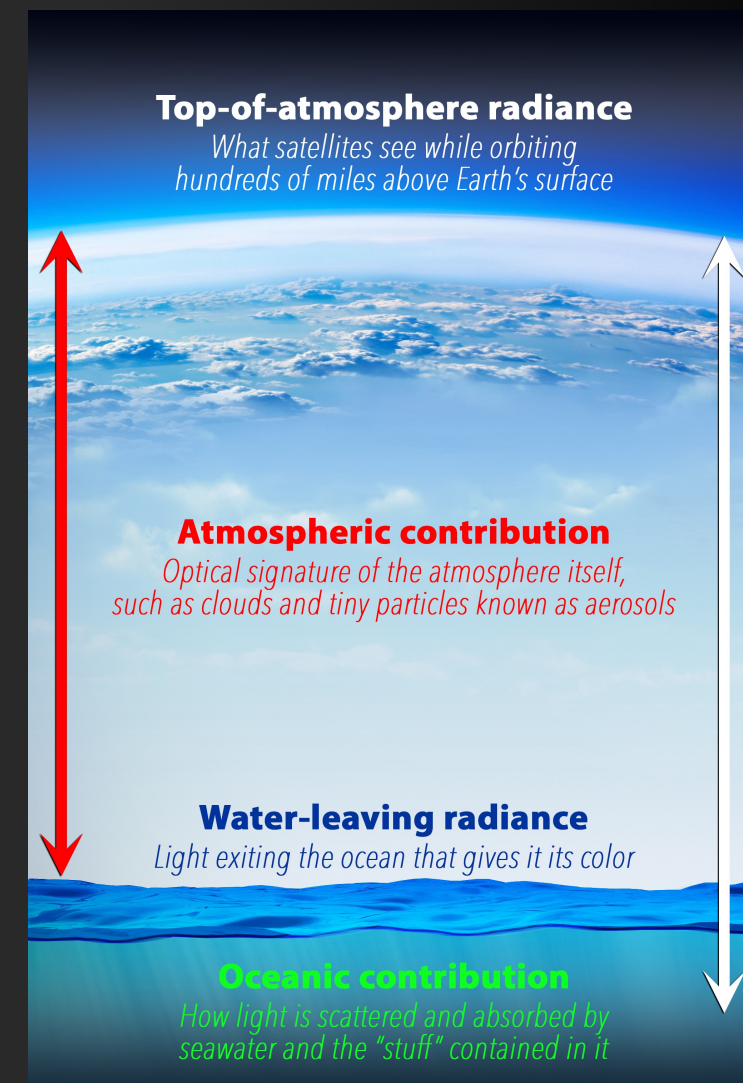
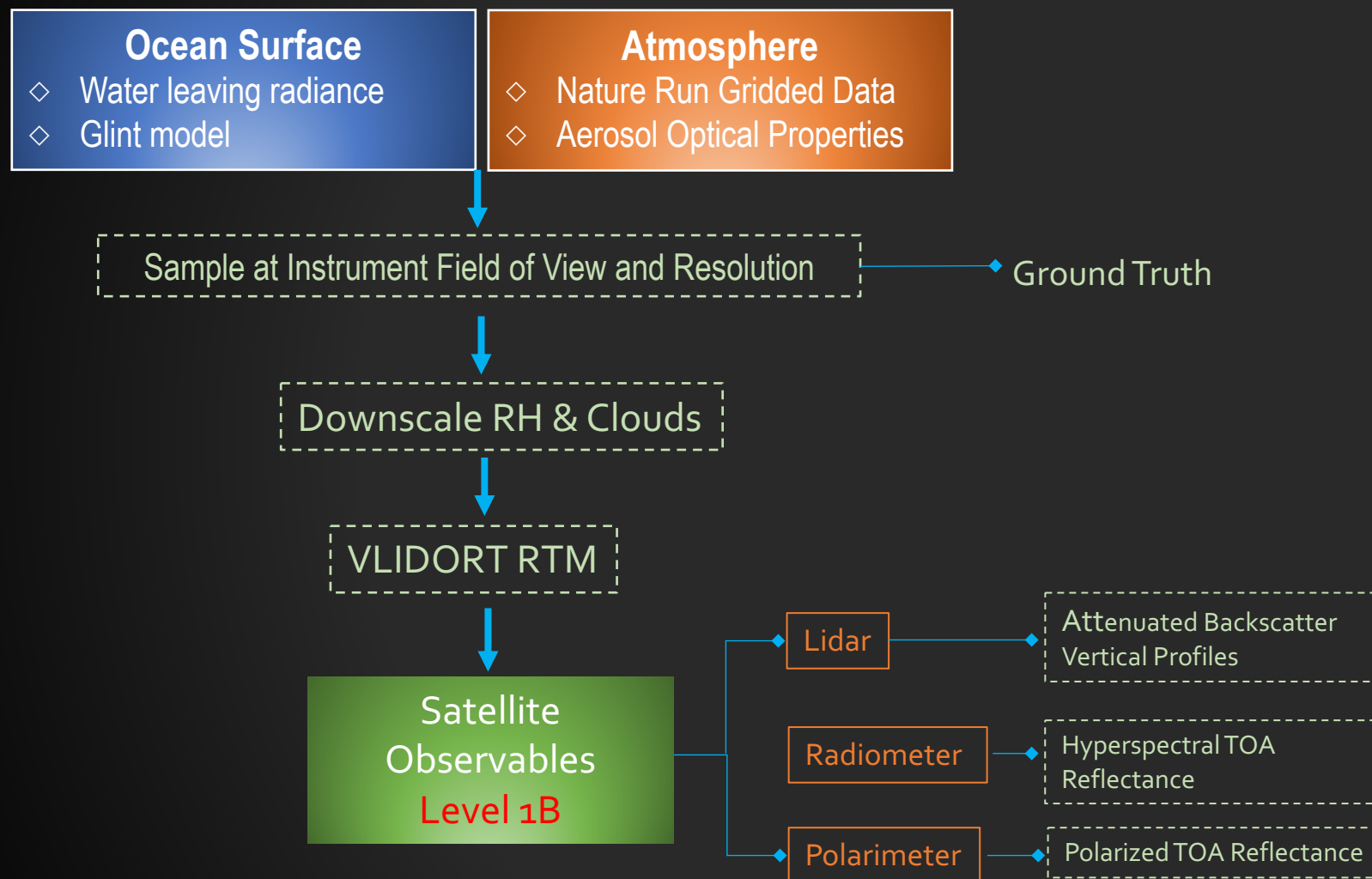
- Dynamic ocean model containing:
 - multiple ocean phytoplankton groups
 - particulate detritus
 - particulate inorganic carbon (PIC)
 - chromophoric dissolved organic carbon (CDOC)

- Biogeochemical constituents were coupled to a global ocean circulation model
- Distributions of ocean optical constituents were coupled with a radiative transfer model OASIM to estimate water-leaving radiances at 1 nm spectral resolution

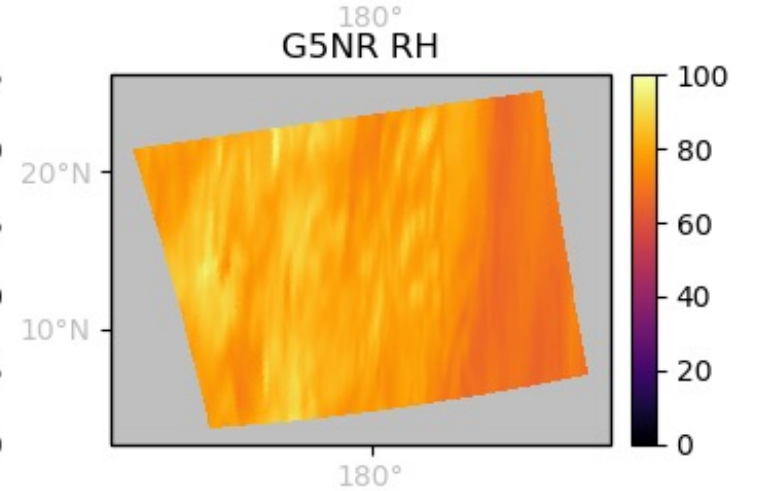
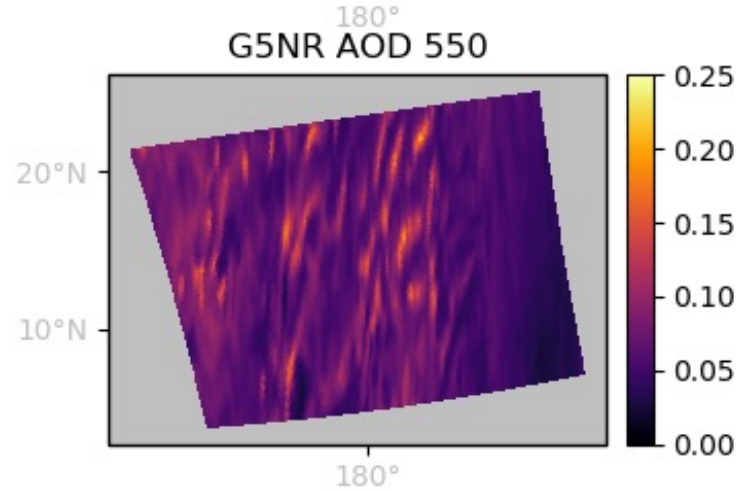
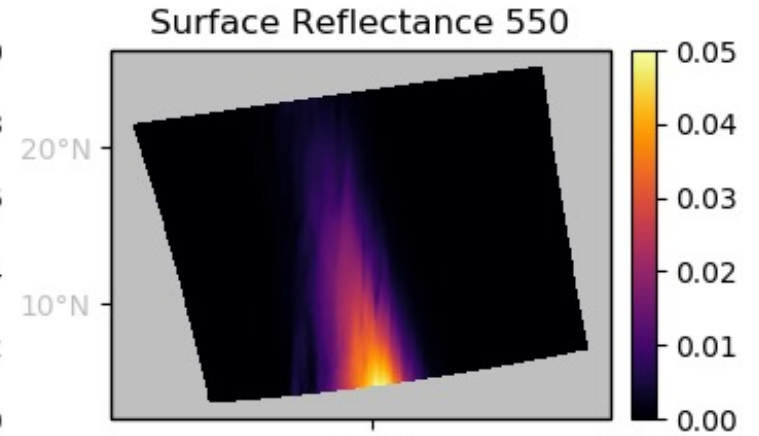
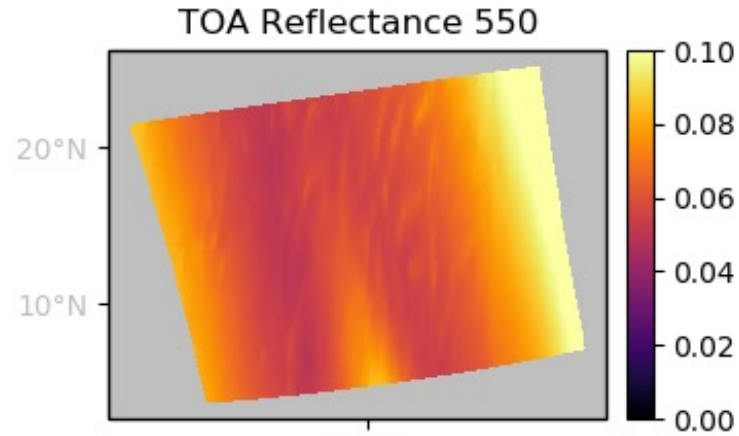
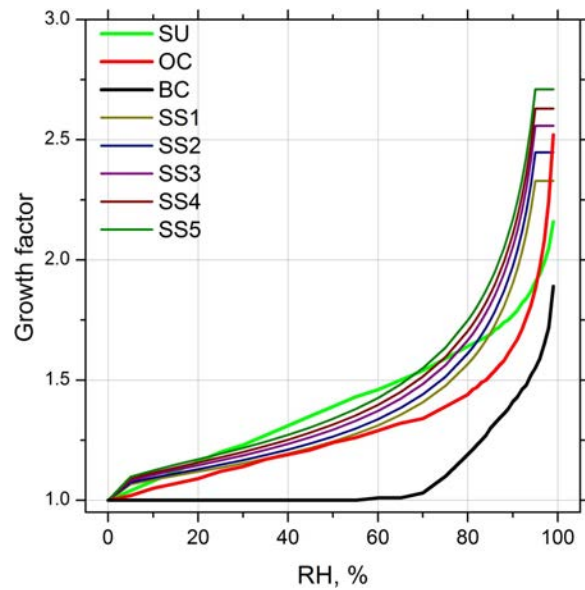
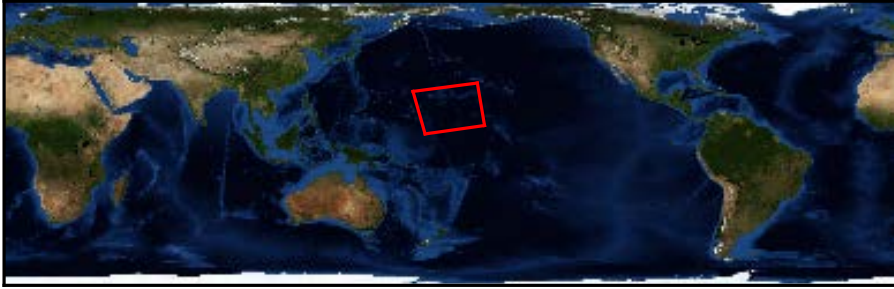
Gregg & Rousseaux, Frontiers in Marine Science (2017)



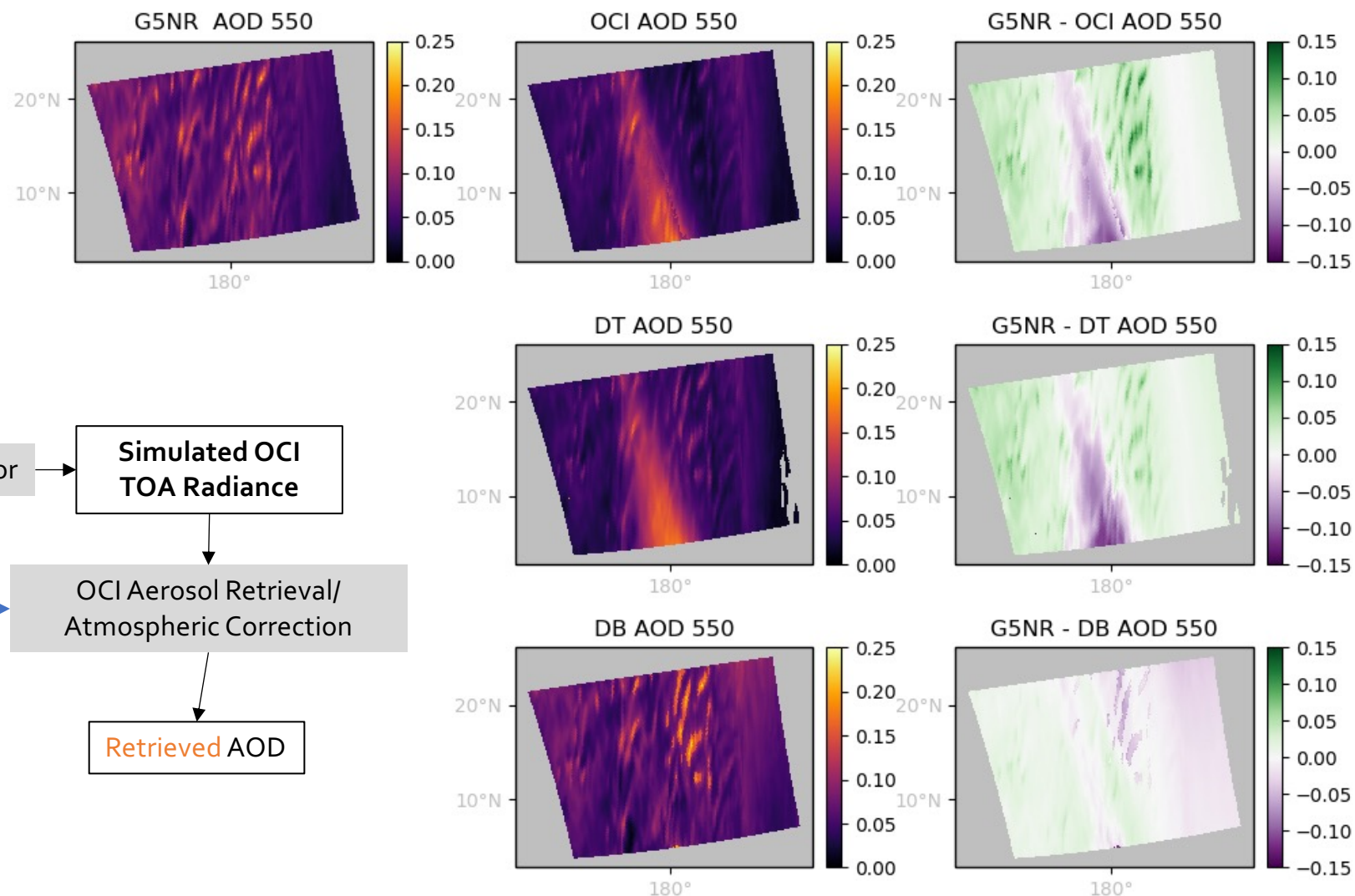
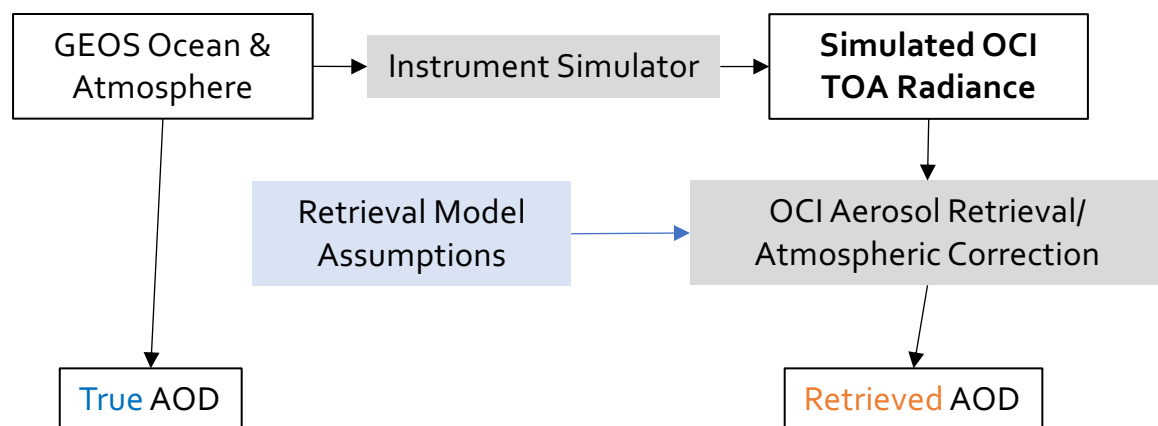
Level 1 Measurement Simulators



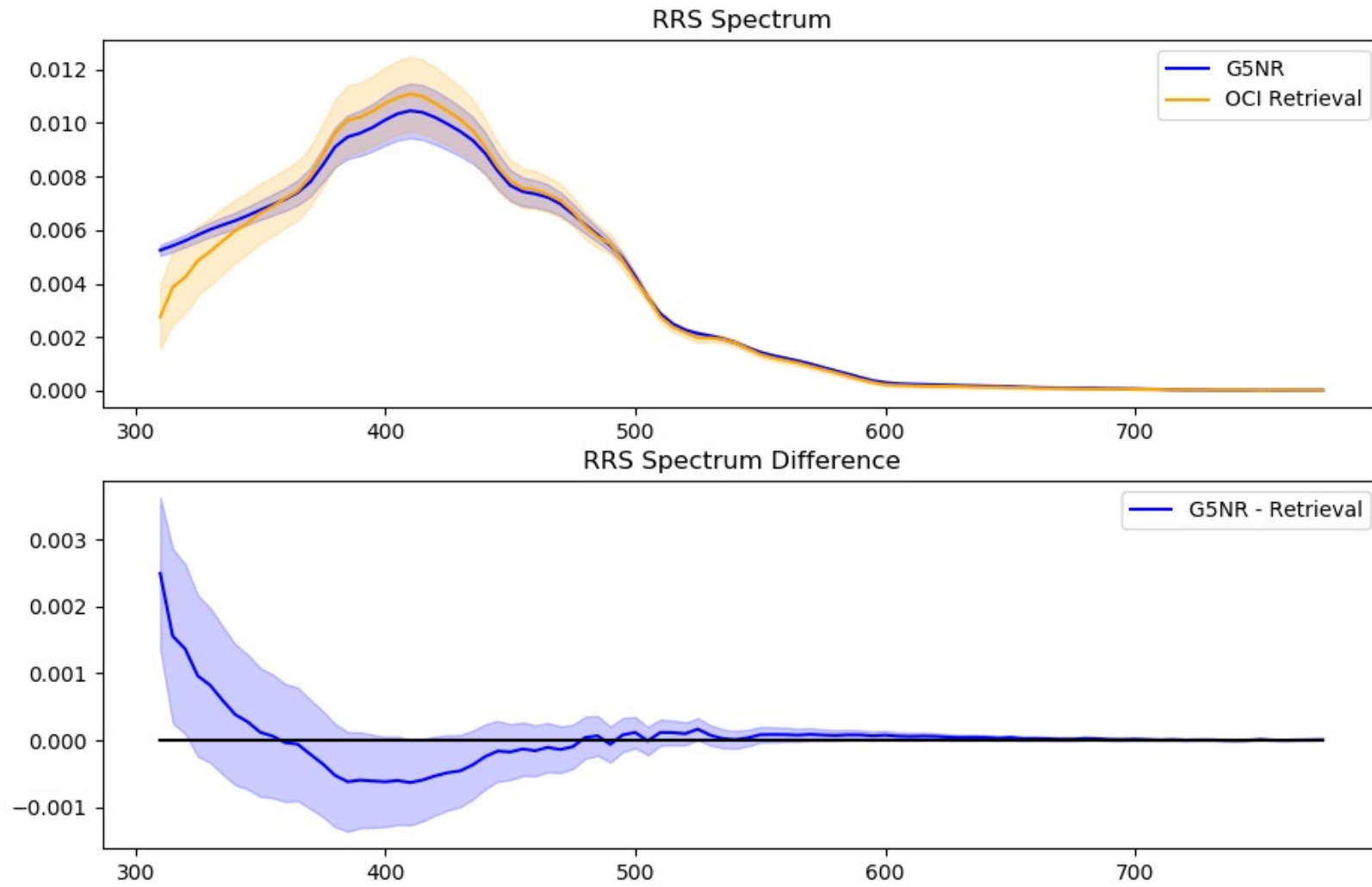
Simulated PACE L1B Granule



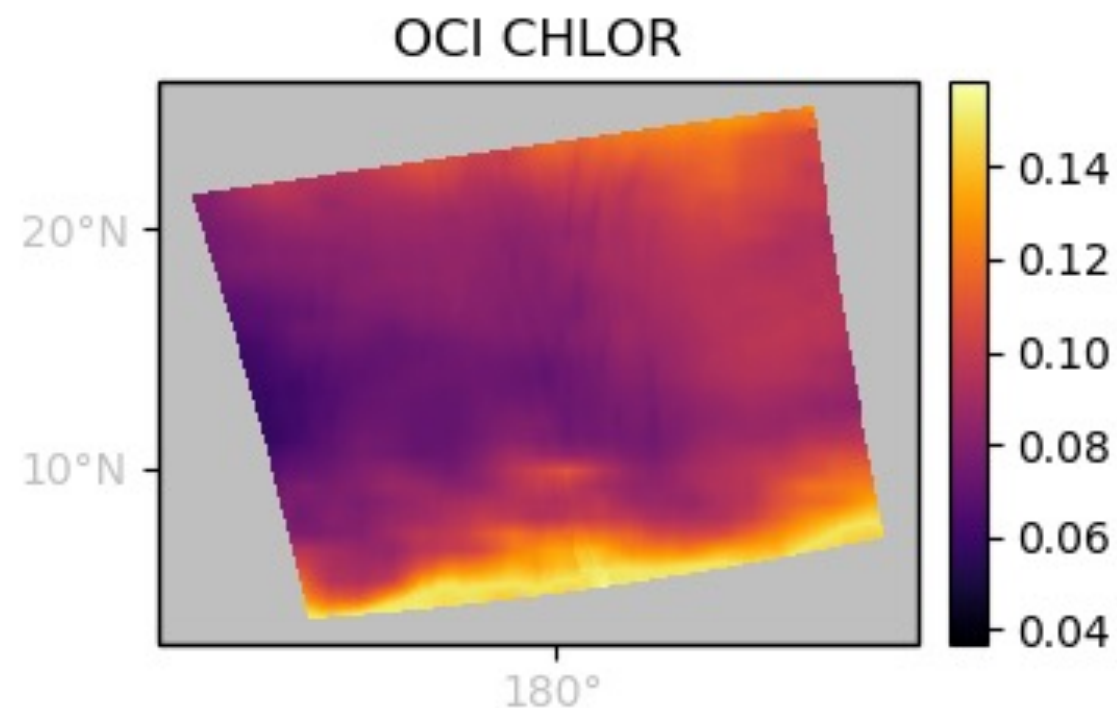
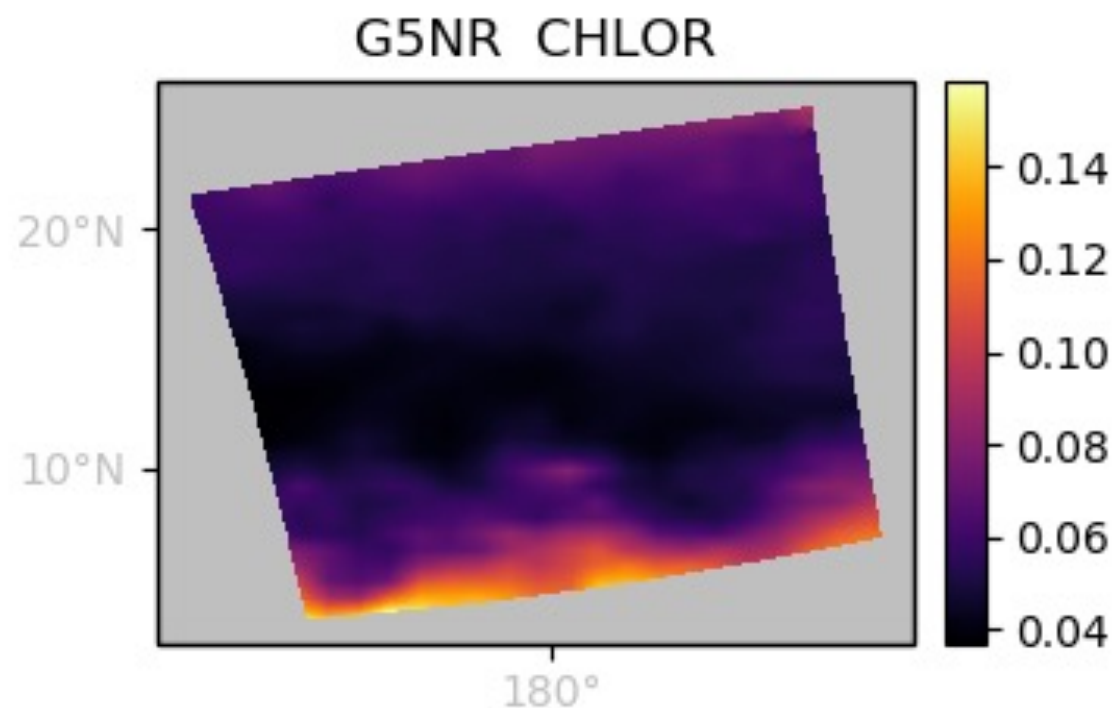
Application to OCI Aerosol Algorithms



Ocean Color Retrieval

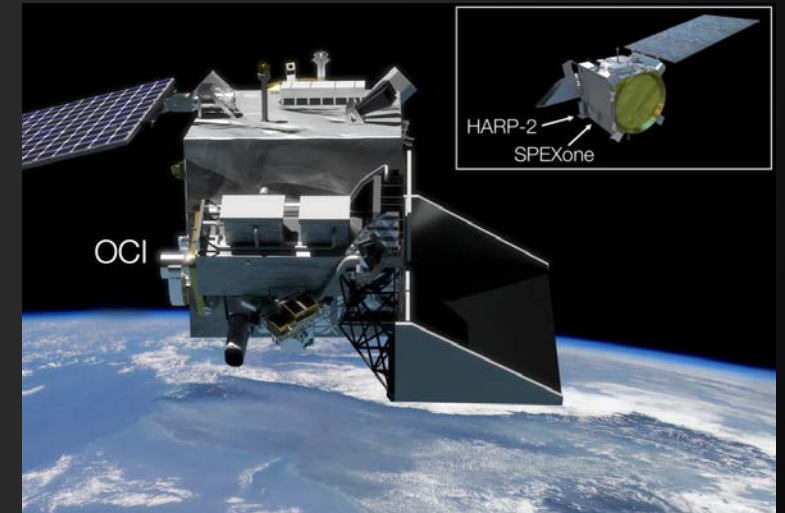


Chlorophyll Retrieval



PACE Contributions to Aerosol Data Assimilation

by Ocean Color Instrument and Polarimeters





Challenges of Aerosol Data Assimilation

□ State representation

- Multiple 3D concentrations
 - ✓ Mass
 - ✓ Number (modal schemes)
 - ✓ Bin sizes (sectional schemes)
- Number of tracers: tens to hundreds

□ Emissions

- Dynamic: dust, marine, biogenic aerosols
- Remotely sensed: biomass burning
- Inventories: anthropogenic
- *Emission estimation* is critical for producing an unbiased model needed for DA

□ Observation operators

- Intrinsic aerosol optical properties needed for assimilation of remotely sensed data
 - Mass extinction coefficient, single scattering albedo, phase matrix
- These are often poorly known but assumed to be known due to identifiability issues:

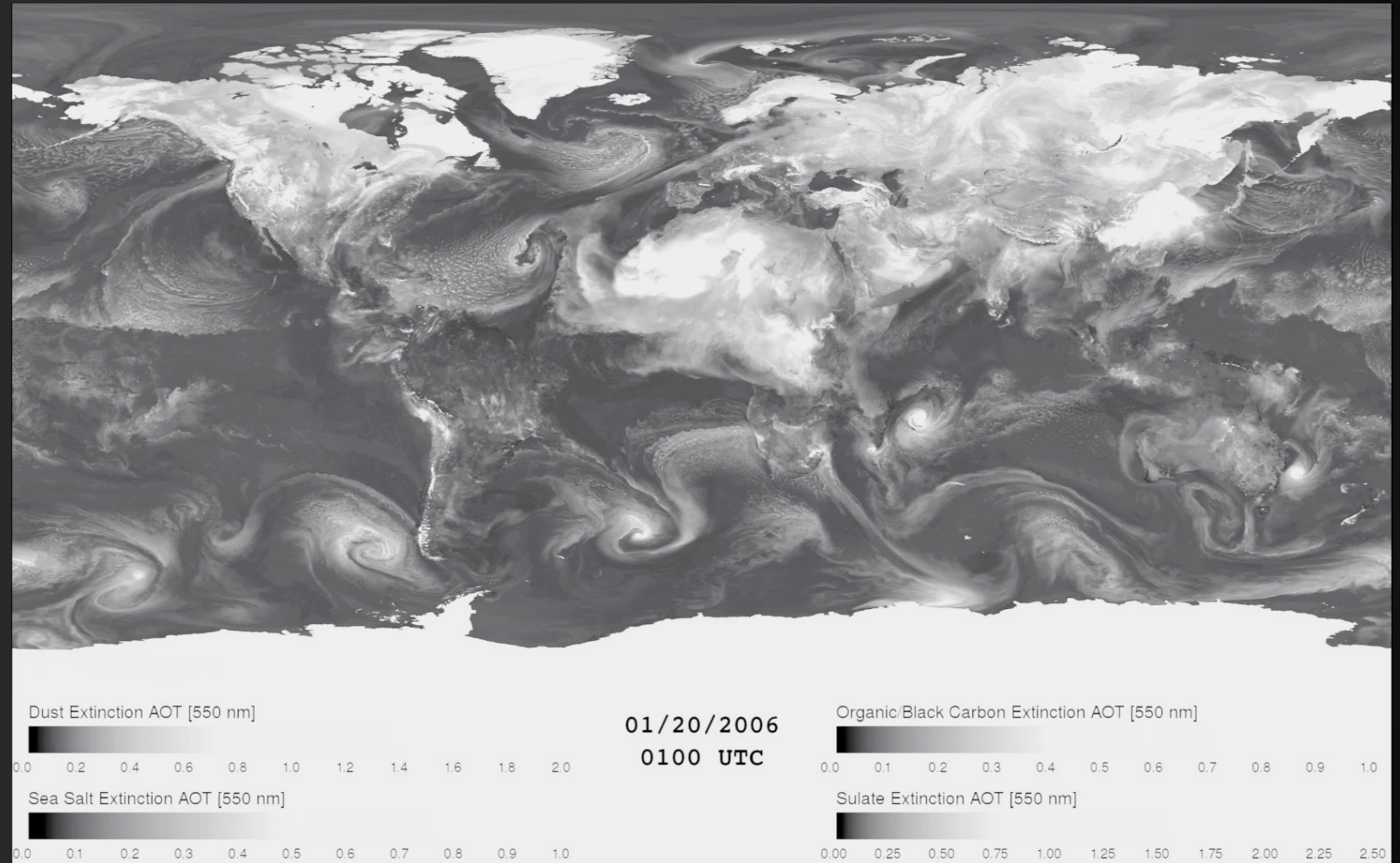
$$\tau = \beta \bullet M$$

- Joint estimation of extensive and intensive properties will be necessary for reconciling a very diverse observing system (multi and hyper spectral, passive/active sensors)

Aerosol Speciation

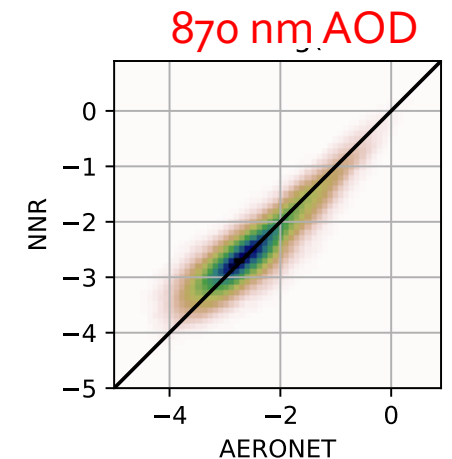
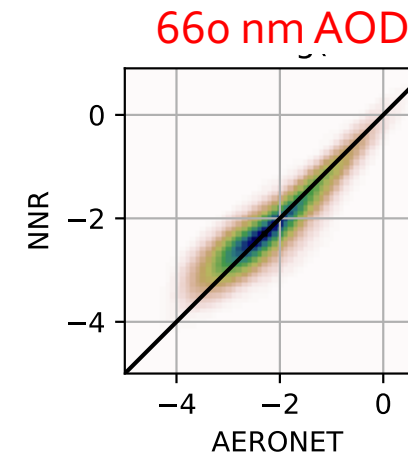
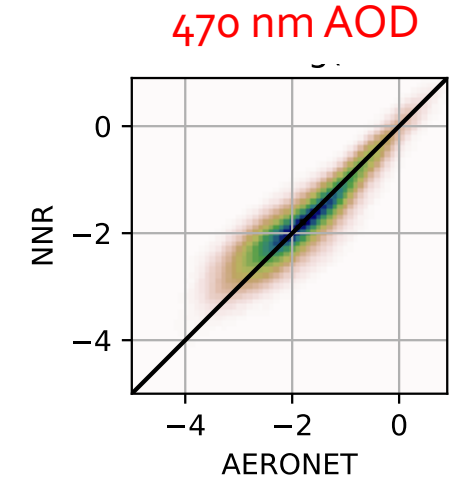
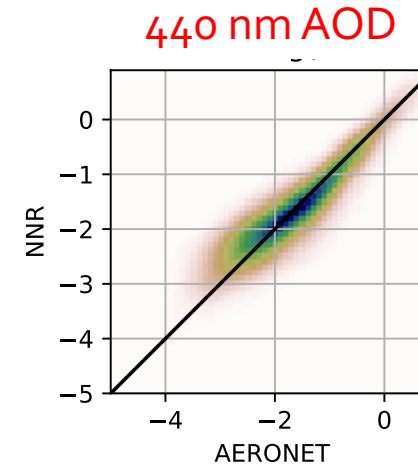
Aerosol Optical Depth (AOD) is the most commonly available observable used for DA

- Vertically integrated mass weighted by extinction coefficient, summed over multiple species: *low observability*
- Single-channel AOD has little impact on speciation
- hyperspectral AOD measurements such as those provided by **PACE OCI** will permit the DA process to adjust the model speciation
- PACE multi-angle, multi-channel polarimeters will bring much needed information content such as size distribution, index of refraction



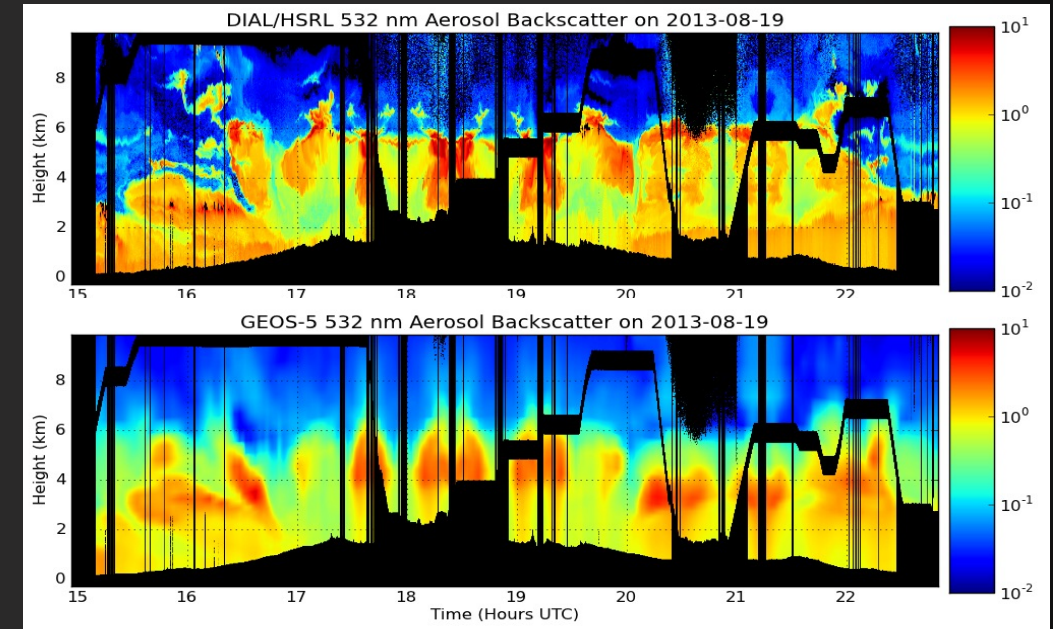
Observing System Homogenization

- Currently assimilating AOD from AERONET, MODIS (VIIRS, geostationary in development)
- AERONET provides the calibration reference
- Originally developed Neural Net algorithm for bias correction of physical retrievals
- Currently, multi-channel Neural Net Retrieval (NNR) trained on AERONET
- Multi-channel AOD derived from multi-channel *Level 2 Reflectances*, no dependency on *aerosol model*



Aerosol Observing System, cont.

- 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
 - HSRL lidar provides (calibrated) particulate backscatter
 - Linear & local obs operator

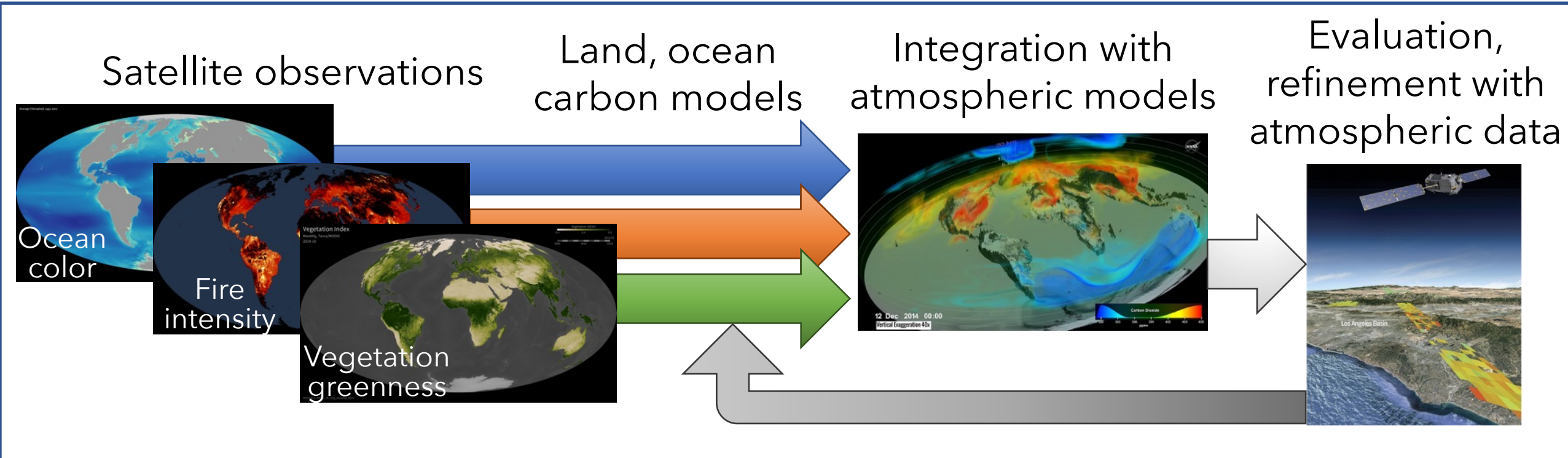




PACE Contributions to Carbon Cycle Studies

By Ocean Color Instrument

Integrated carbon cycle modeling at NASA



- NASA specializes in observation-driven modeling
- Models play role of integrating across spatial scales, observation types
- Model provide estimates of key unobserved (or under-observed) variables (e.g. biomass, flux)
- Ability to provide low latency estimates of carbon in land, atmosphere, oceans
- Complement national-level inventories with higher resolution CO₂, CH₄ information
- Ability to predict future conditions and connect ecosystem dynamics to climate impacts



Summary

- Main Components of an Earth System Model and potential **PACE contributions**
 - Numerical Weather Prediction
 - Atmospheric Constituents
 - Aerosols
 - Greenhouse gases
 - Reactive gases
 - Ocean
 - Physical ocean: salinity, temperature, currents
 - Sea-ice
 - Ocean bio-geochemistry
 - Land surface
 - Hydrology
 - Vegetation

