Progress in Aerosol OSSE, Data Assimilation and ACE

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NASA/Goddard Space Flight Center
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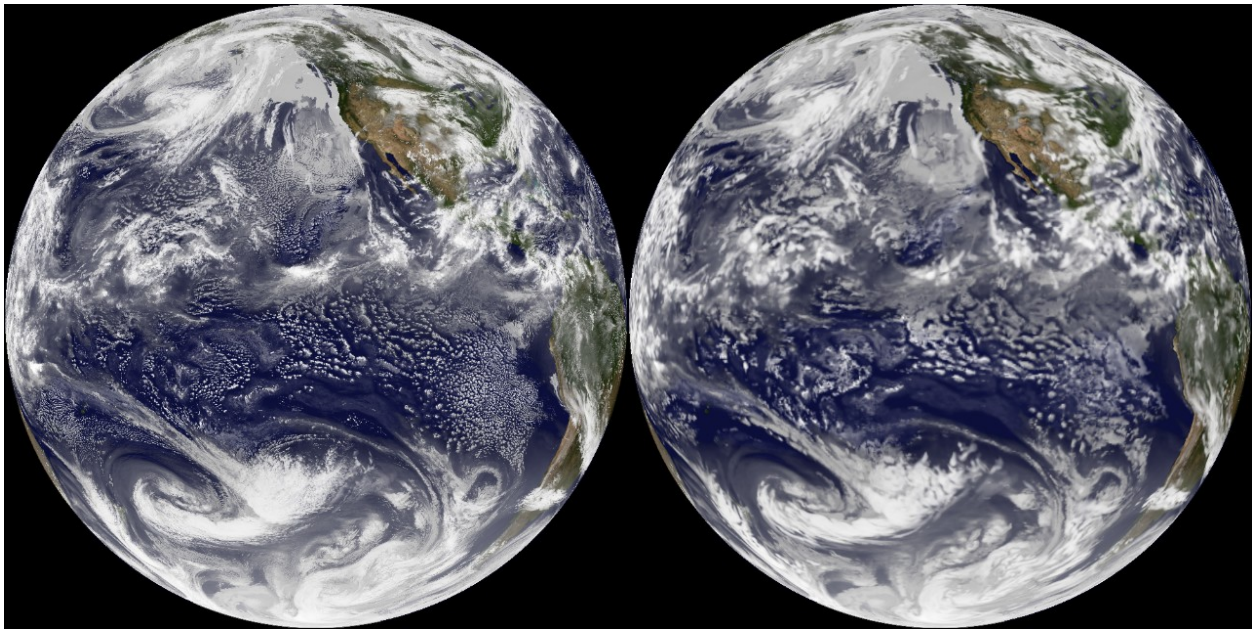
Outline

- Introduction
- Current and emerging capabilities
  - Aerosol Forecasting & Re-analysis Capabilities
  - Data assimilation: State & Source Estimation
  - Global Aerosol Observing System
  - Observing System Simulation Experiments (OSSEs)
- Applications to ACE
  - Pre-launch: OSSE
  - Post-launch: Level 4, Level 2a products, IESA

Scope

- Global Domain
- Resolutions:



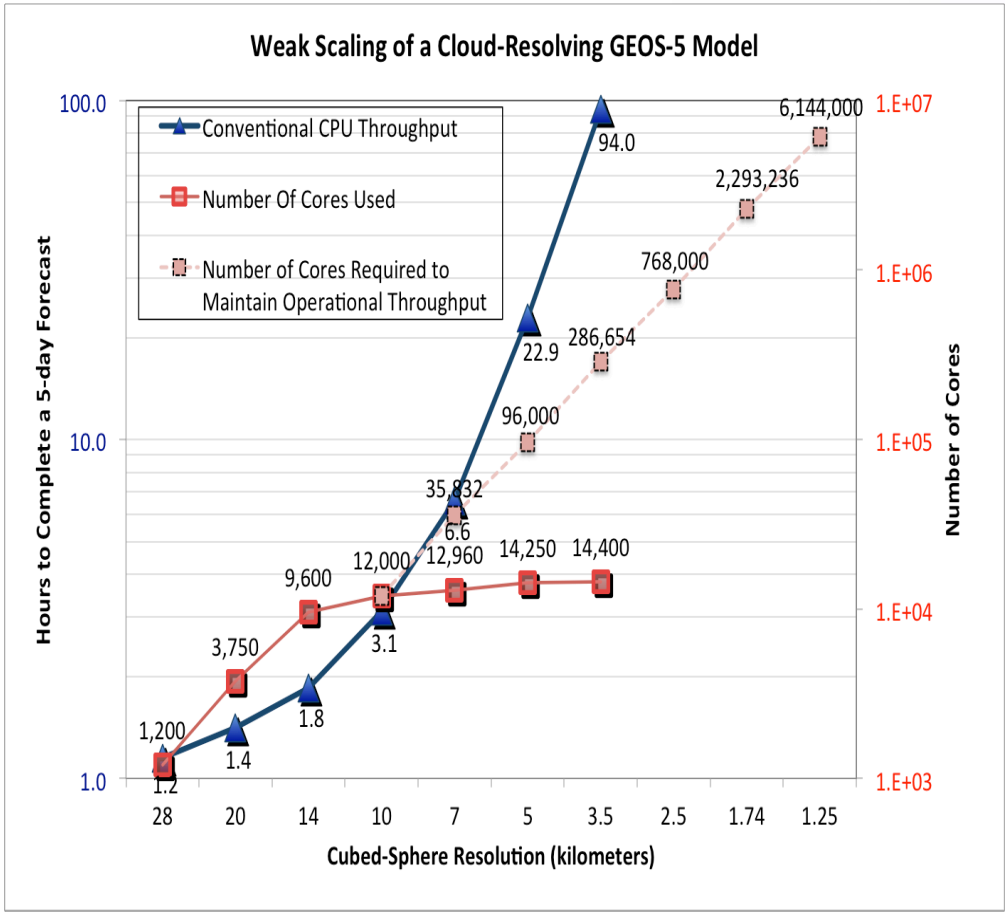
3.5 km

25 km

Motivation for Accelerators

Weak Scaling of GEOS-5

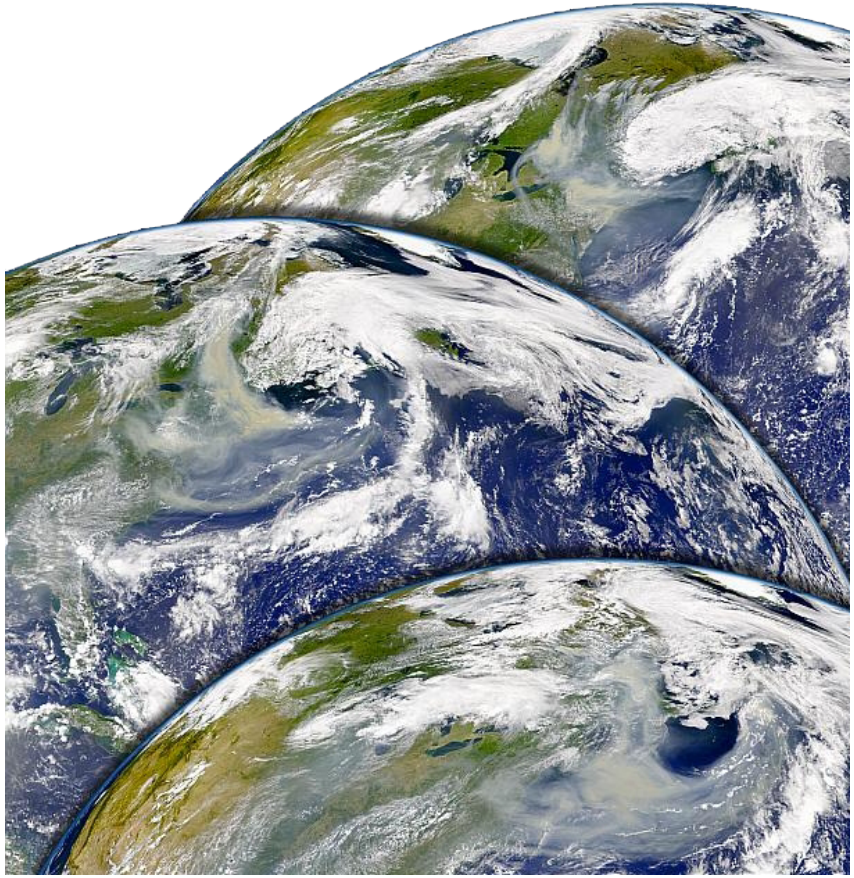
- Global models are reaching resolutions of 10- to 1-km
- This requires hundreds of thousands of conventional processors
- At current cloud-permitting resolutions (10- to 3-km) required scaling of 300,000 cores is reasonable (though not readily available)
- **To get to global cloud resolving (1-km or finer) requires order 10-million cores**
- Weak scaling of a global cloud-permitting GEOS-5 model indicates need for accelerators
- ~90% of those computations are in the dynamics



Evolution of Global Constituent Modeling

- **First Generation:**
  - Off-line Chemical Transport Models
  - Transport driven by assimilated meteorology
- **Second Generation:**
  - Bulk: mass only
  - On-line transport within GCM
  - Dynamical-Radiative Feedbacks
  - Transport constrained by meteorological assimilation
- **Third Generation:**
  - Modal (Mass,Number) or bin-resolved
  - Aerosol-cloud microphysics
  - Aerosol modulation of snow albedo
  - Aerosol-chemistry coupling
  - Aerosol coupling to biogeochemistry
  - Coupling to wind wave models for better sea-spray aerosol emissions
  - etc.

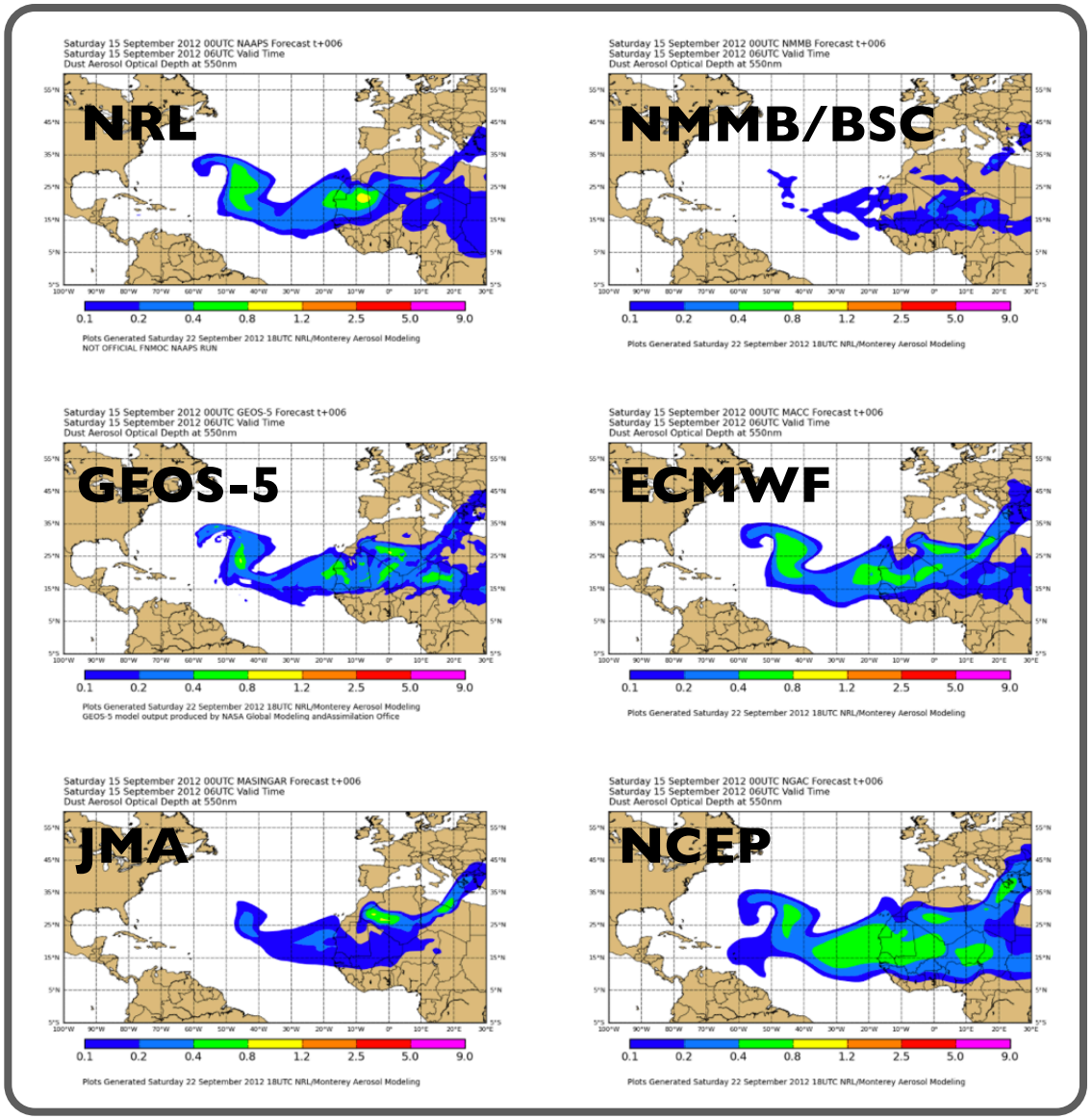
International Cooperative for Aerosol Prediction (ICAP)



- ICAP is an emerging collaboration of "operational" aerosol forecasters and data providers to coordinate and improve aerosol prediction
- ICAP goals
  - Communication and collaboration between operational prediction centers
  - Communication and collaboration between model developers and data providers
  - Develop metrics for evaluating skill of model forecasts (similar to NWP community)
  - Develop techniques for aerosol data assimilation
  - Develop techniques for ensemble model forecasting

ICAP Multi-model Ensemble

- Participation from all major operational centers: NRL, NCEP, NASA, ECMWF, JMA, UKMO
- Participation from all major data providers: ESA, EUMETSAT, JAXA, NASA, NESDIS
- ICAP workshops
  - Observability, Monterey, CA, April 2010
  - Verification, Oxford, UK, Sept. 2010
  - Ensembles, Boulder, CO, May 2011
  - Sources & Sinks, Frascati, IT, May 2012
  - Observabiloty, Tsukuba, Japan, Nov 2013
- Two workshop write-ups in BAMS
- ICAP Multi-Model Ensemble; ACP paper currently in discussion

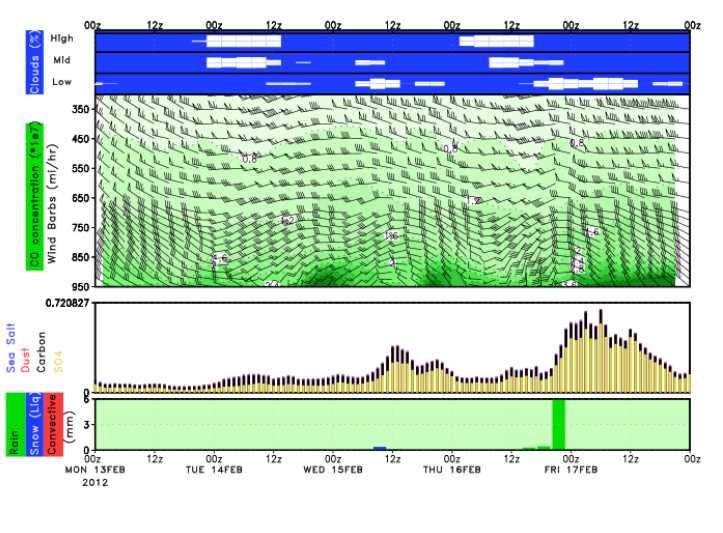


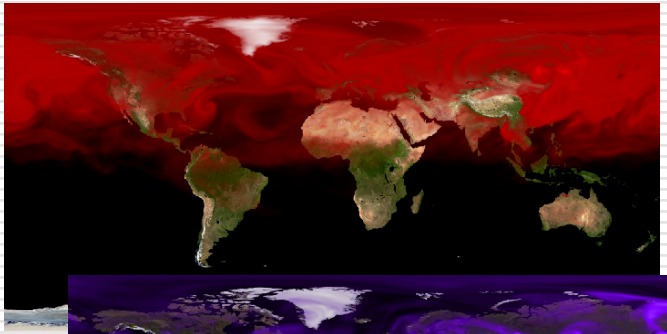
ICAP Multi-Model Ensemble Dust Forecast

GEOS-5 Forecasting Support

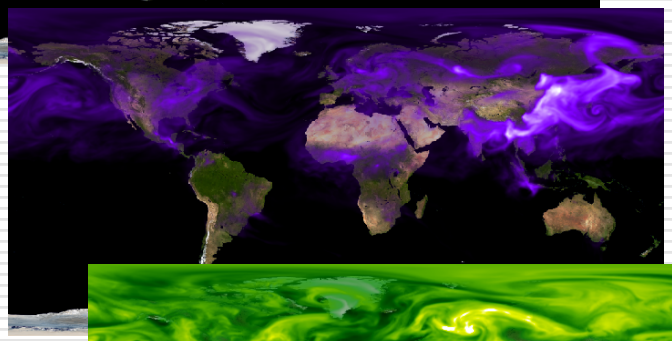
DISCOVER-AQ

- Global 5-day chemical forecasts customized for each campaign
  - O3, aerosols, CO, CO_2, SO_2
  - Resolution: Nominally 25 km
- Driven by real-time biomass emissions from MODIS
- Assimilated aerosols interacts with circulation through radiation

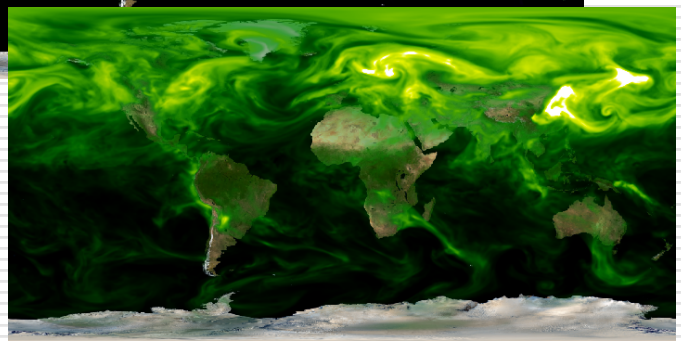




CO



Smoke



SO_4

http://gmao.gsfc.nasa.gov/forecasts/

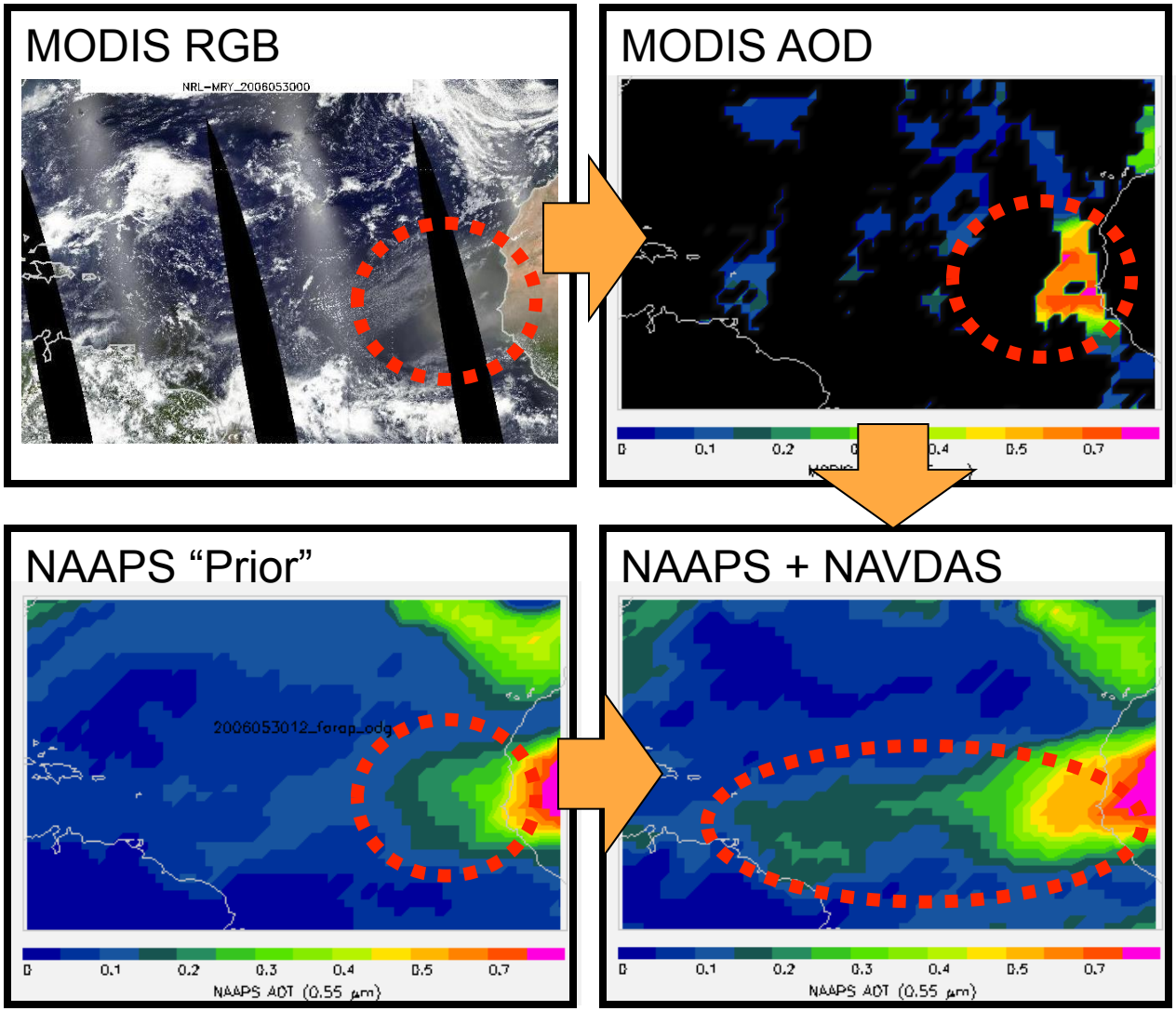
GEOS-5 Reanalysis Activities

Name	Nominal Resolution	Period	Aerosol Data	Available
MERRA-1	50 km	1979-present	NONE	now
MERRAero	50 km	2002-present	MODIS C5	now
FP for Inst. Teams	50 km	1997-	MODIS C5	In progress
NCA	25 km	2010-11	MODIS C5, MISR	Now
MERRA-2	50 km	1979-present	AVHRR, MODIS C5, MISR, AERONET	Q4 2014

Monitoring Atmospheric Composition and Climate- Interim Implementation

- 36-partner Collaborative Project, funded by European Union FP7
- Started in November 2011 with expected completion in July 2014
- Prototype for the operational Copernicus Atmospheric Service (follow-on of MACC project)
- Providing air quality regional forecasts and **global atmospheric composition forecasts and reanalysis** in support of Europe's air quality policies and health aspects

Navy Global Aerosol Forecasting



- **Navy Aerosol Analysis and Prediction System (NAAPS) operational since 2005**
- **Navy Variational Data Assimilation System for AOD (NAVDAS-AOD) Operational at FNMOC from September 2009 (MODIS over ocean)**
- **Global MODIS is assimilated operationally as of February 2012**
- **J.L. Zhang et al., "A System for Operational Aerosol Optical Depth Data Assimilation over Global Oceans", JGR 2008.**

Data Assimilation

State, Source & Parameter Estimation

- Prognostic equation: mass conservation

$$\frac{\partial \rho_a q}{\partial t} + \nabla \cdot \rho_a \mathbf{u}\mathrm{q} + \mathrm{T(q)} = \mathrm{P} - \mathrm{L}$$

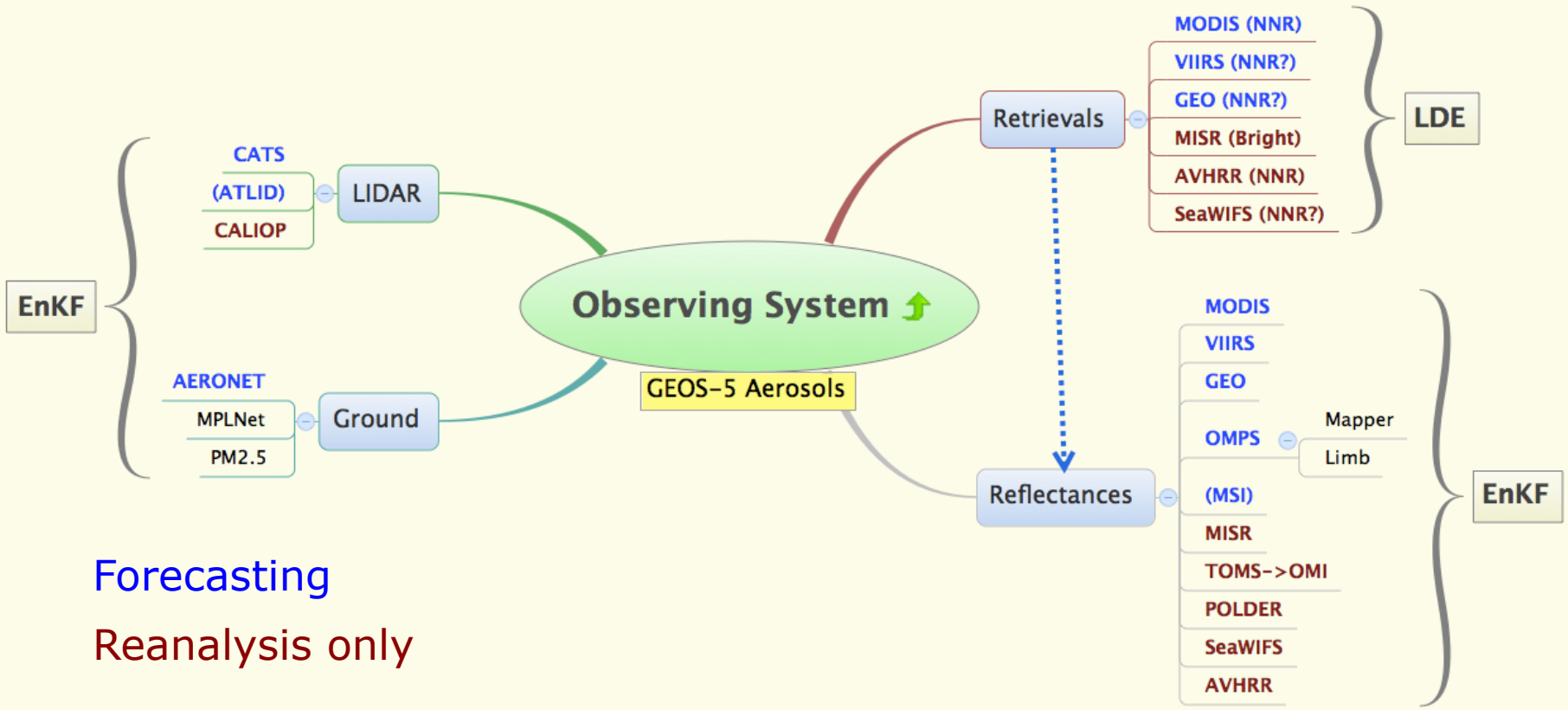
- Observations can be used to constrain:
  - Tracer state, e.g., mixing ratio *q*, number conc.
  - Emissions (included in *P*)
  - Generic model parameters
  - Model/observation biases

Measurement Equation

$$y^o = h(q^t; p) + \epsilon^o$$

y^o	observation vector
h	nonlinear observation operator
p	observation operator parameters
q^t	true state
ϵ^o	observation error

Aerosol Observing System



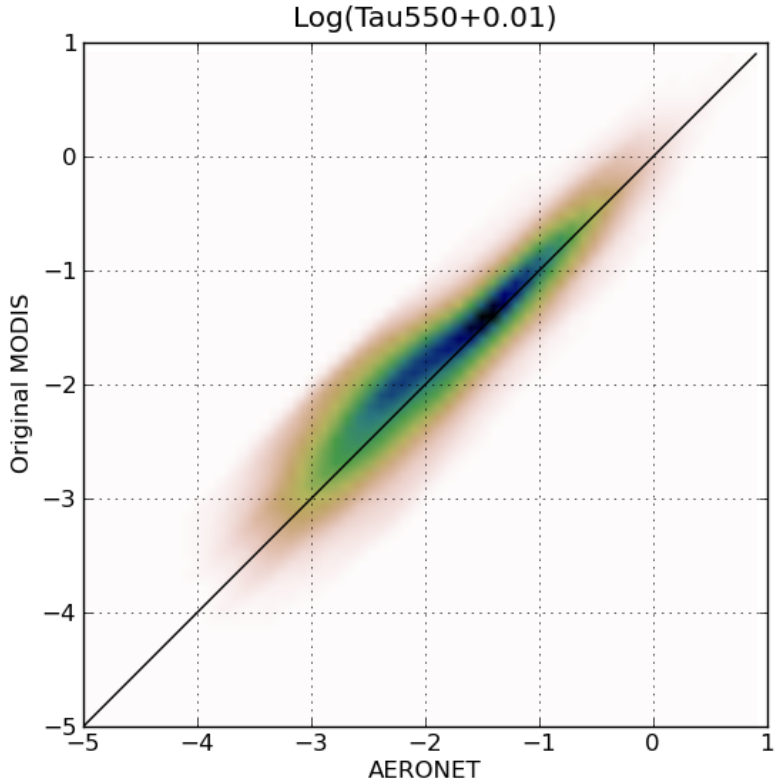
Forecasting

Reanalysis only

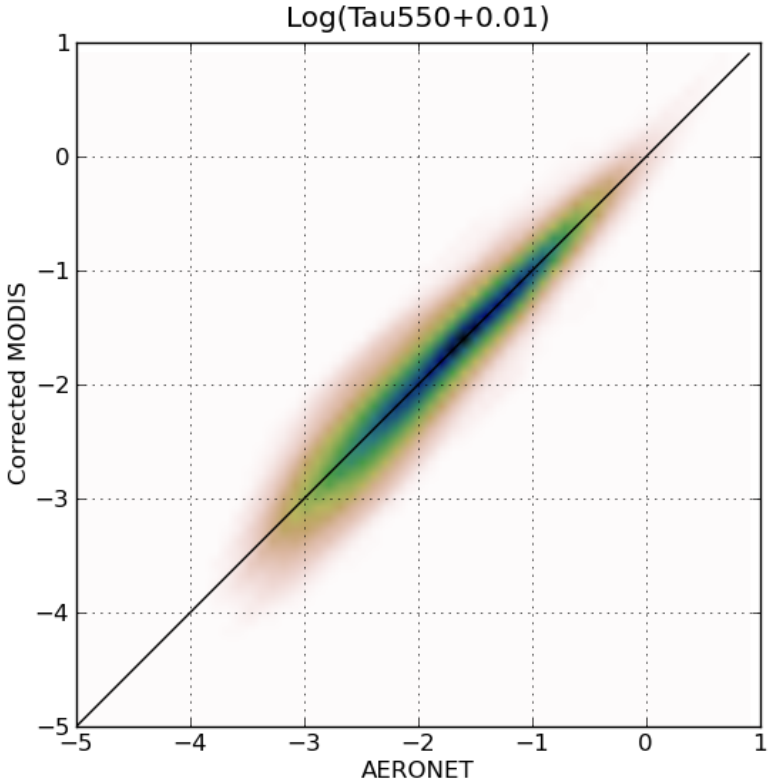
Aerosol Data Assimilation in GEOS-5

Observational Bias

ORIGINAL MODIS AOD



BIAS CORRECTED AOD



Optimal Estimation

- Cost function:

$$J(x) = \left[x - x^b\right]^T \mathbf{B^{-1}} \left[x - x^b\right] + \left[y^o - h(x)\right]^T \mathbf{R^{-1}} \left[y^o - h(x)\right]$$

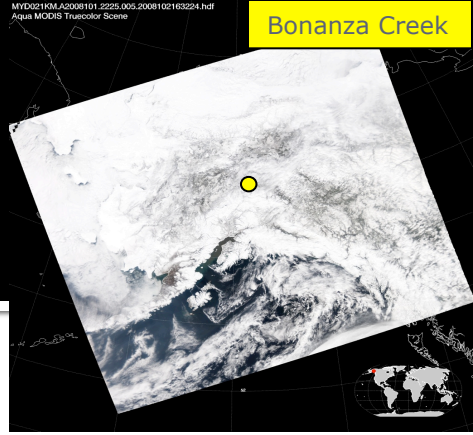
- Control variable x is typically prog variable
- The observation operator involves optical assumptions, *e.g.*,

$$h(x) = \delta\tau = \beta_e(r_e, n_r, n_i) q \rho \delta z$$

Radiance Assimilation vs Retrievals

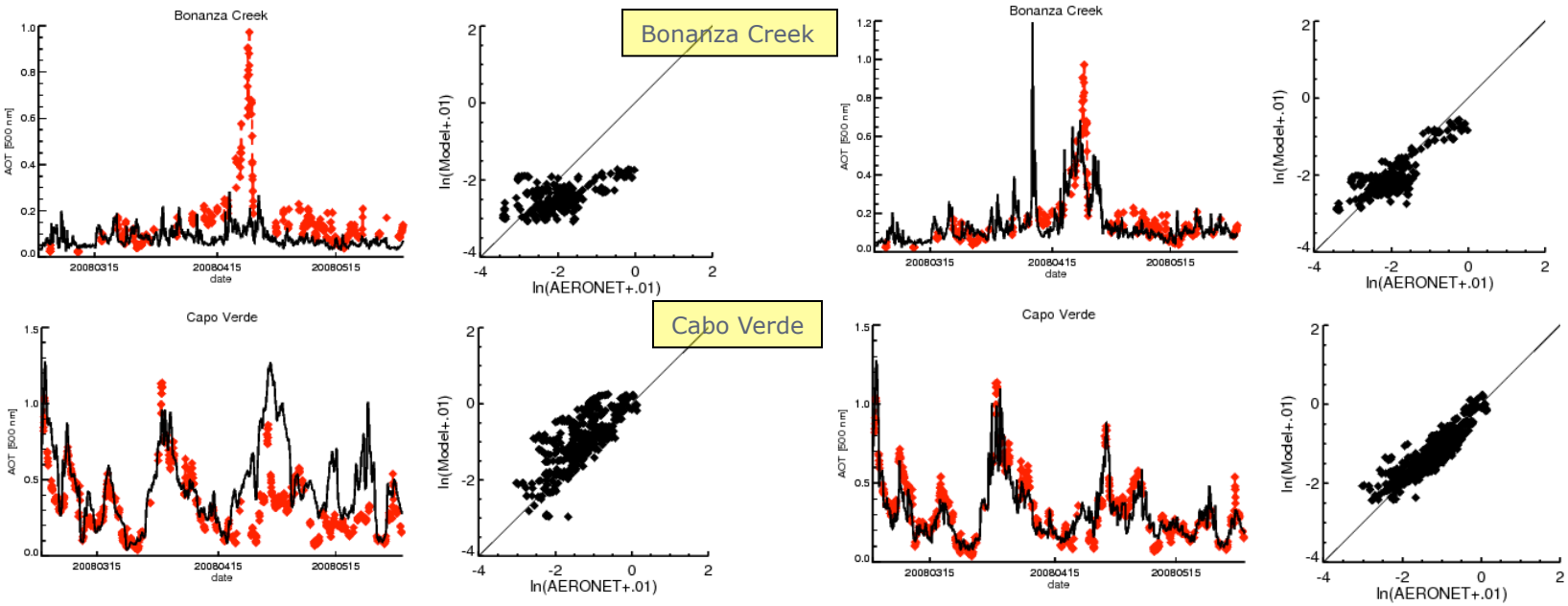
- In DA, model serves as a conveyor of past observations through forecast prior x^b
  - Smallest change from x^b that matches observations within specified uncertainty
- Problem is solved multivariately in 3D or 4D
  - In-line RT calculations, usually no LUTs
- The "aerosol model" is implicit in the mixing state and optical assumptions
- Conservation of difficulty:
  - Handling of surface, identifiability issues
  - Lack of adequate information content in observations

Model as a conveyor of Remote Observations



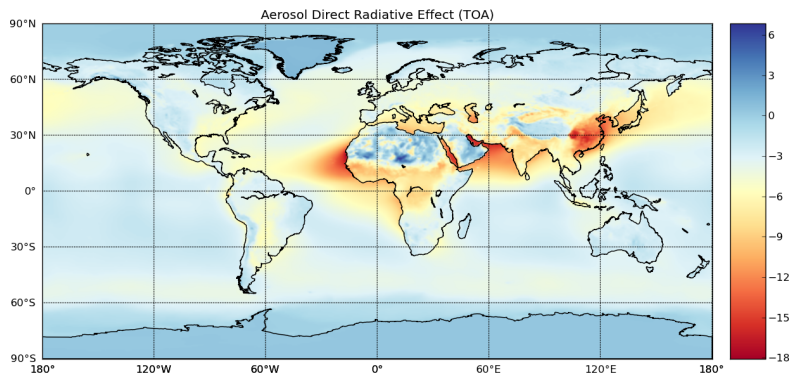
GEOS-5 AOD Without MODIS Assimilation

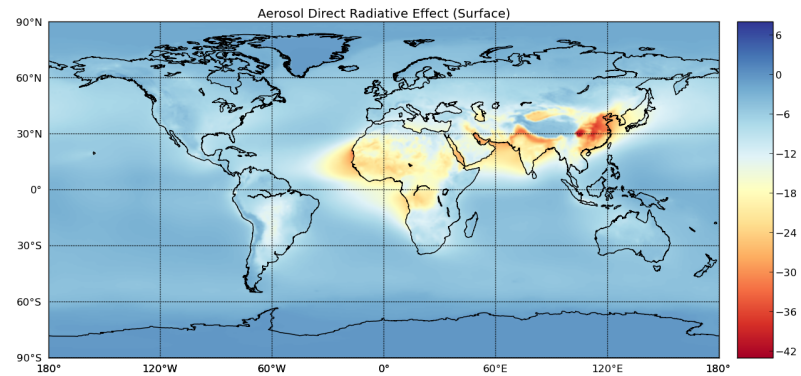
GEOS-5 AOD With MODIS Assimilation



Comparison against independent AERONET ground stations.

Clear-Sky Aerosol Direct Radiative Effect

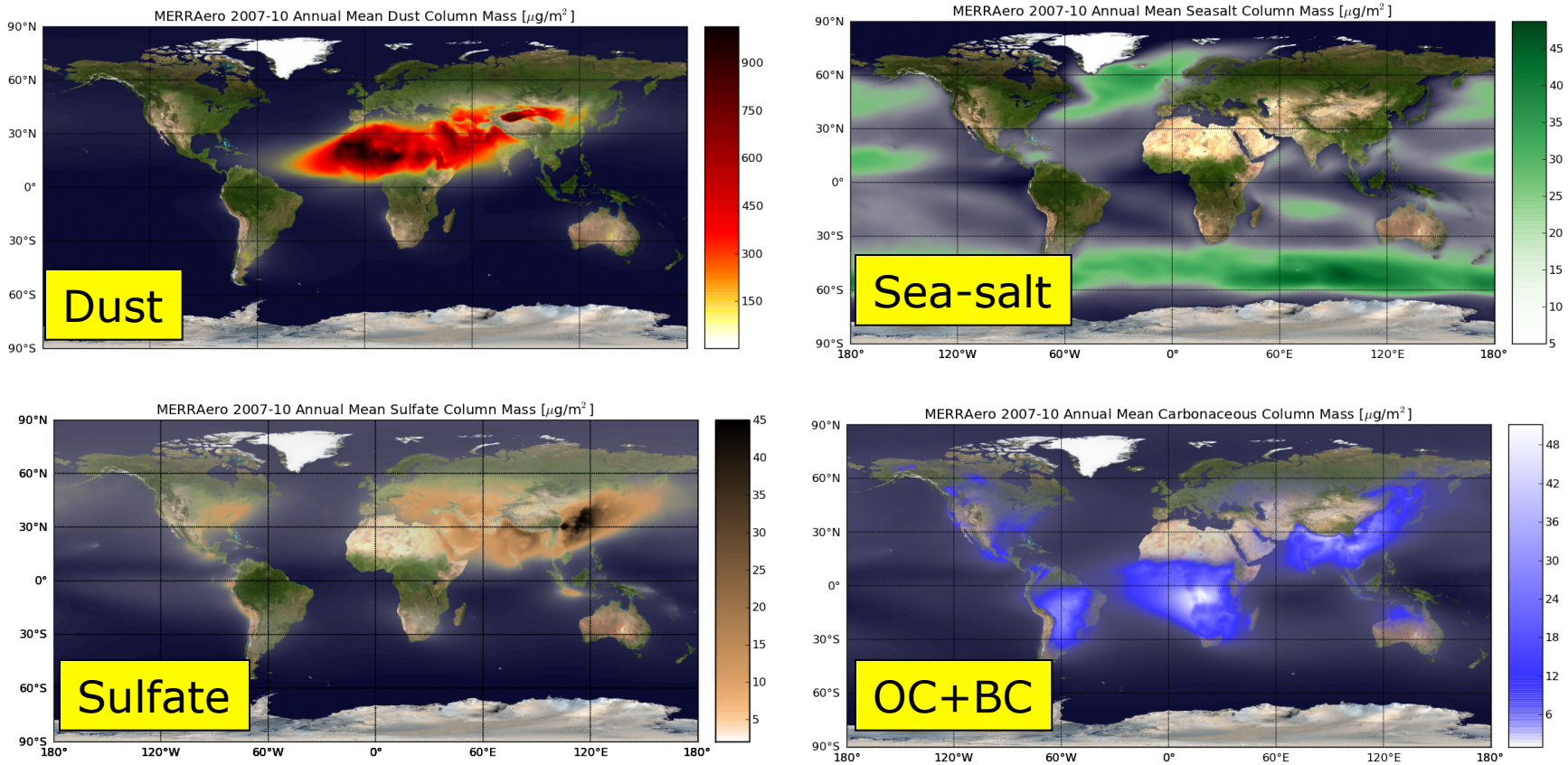




Source	TOA SW DRE Ocean (Land)	Atmos. Ocean (Land)	Surface SW DRE Ocean (Land)
MERRAero	-3.8 (-4.3)	2.8 (6.8)	-6.6 (-11.1)
Other Observational Yu *et al.* (2006)	-5.5 ± 0.2 (-4.9 ± 0.7)	3.3 (6.8)	-8.8 ± 0.7 (-11.8±1.9)
Multi-model Ensemble Yu *et al.* (2006)	-3.4 ± 0.6 (-2.8 ± 0.6)	1.4 (4.4)	-4.8 ± 0.8 (-7.2 ± 0.9)
GEOS-5 (Free)	-3.4 (-2.7)	0.5 (2.8)	-3.9 (-5.5)

$$DRE_{SW} = \left(F^{\downarrow}_{SW} - F^{\uparrow}_{SW}\right)_{Aerosols} - \left(F^{\downarrow}_{SW} - F^{\uparrow}_{SW}\right)_{NoAerosols}$$

Assimilated Aerosol Annual Mean Mass



Speciation potentially adjusted by spectral reflectances

Mass Budget

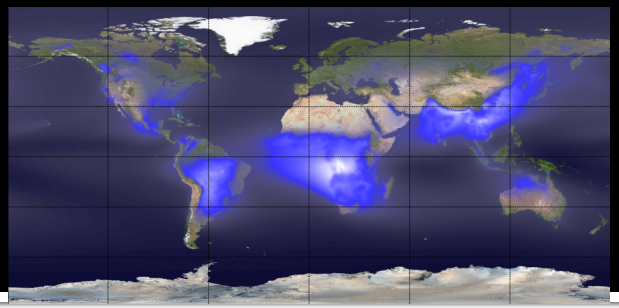
Annual mass budget for an aerosol specie q:

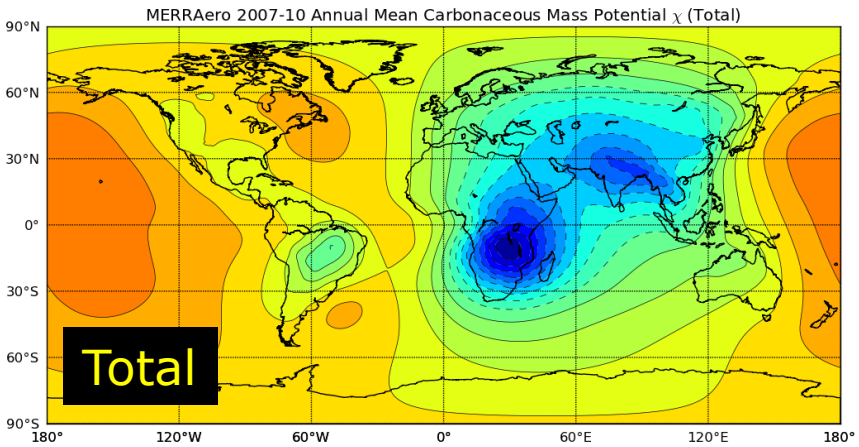
$$\nabla \cdot \overline{\langle \mathbf{u}q \rangle} = \overline{E} + \overline{P} - \overline{L} + \frac{\overline{\langle \Delta q^a \rangle}}{\tau}$$

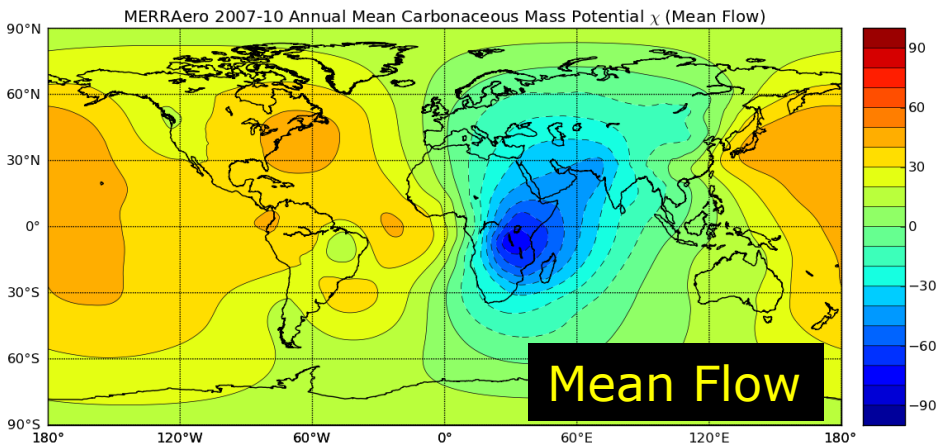
where

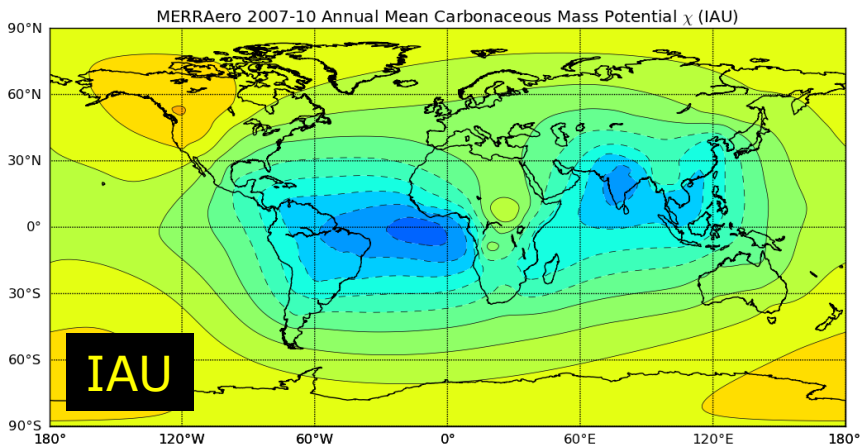
$\mathbf{u}q$	Mass flux
E	Emissions
P	Chemical production
L	Loss processes
Δq^a	Anaysis increments
τ	Analysis interval (3 hours)
$\langle \cdot \rangle$	Mass weighted vertical integral
$\overline{(\cdot)}$	Time average

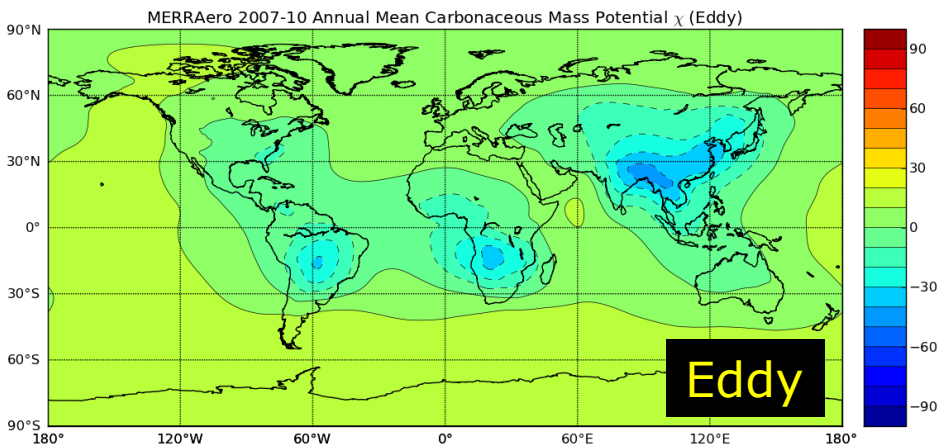
Annual Carbonaceous Flux Potential









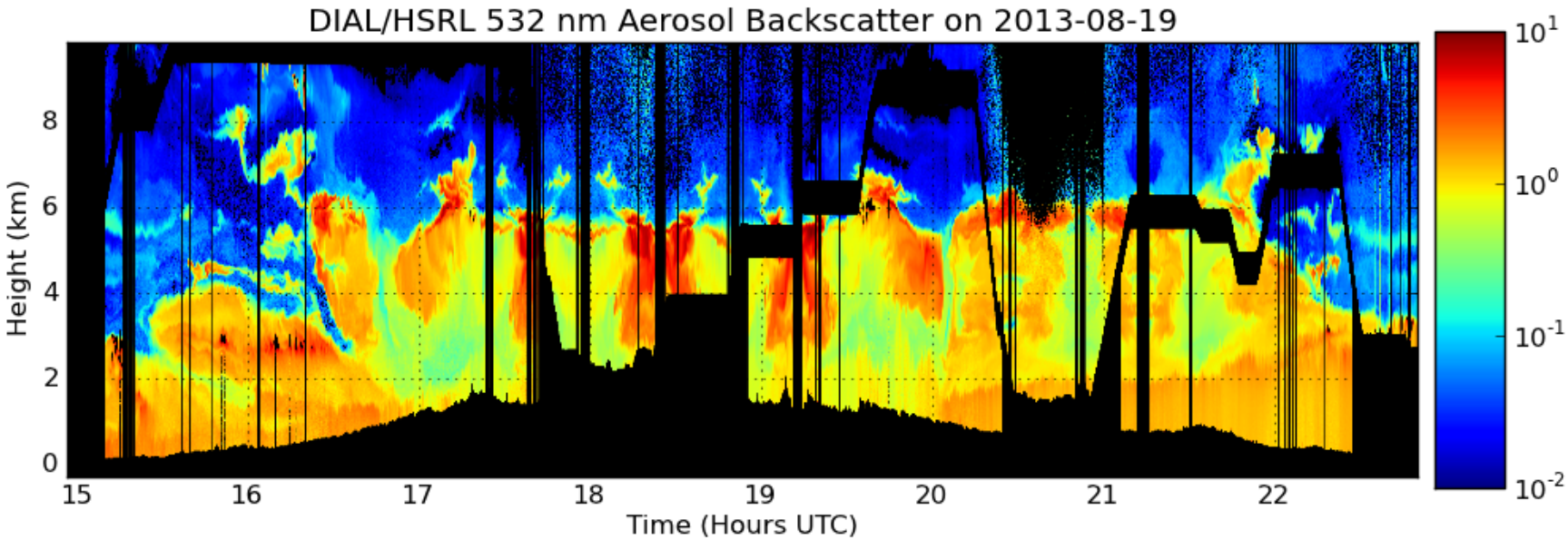


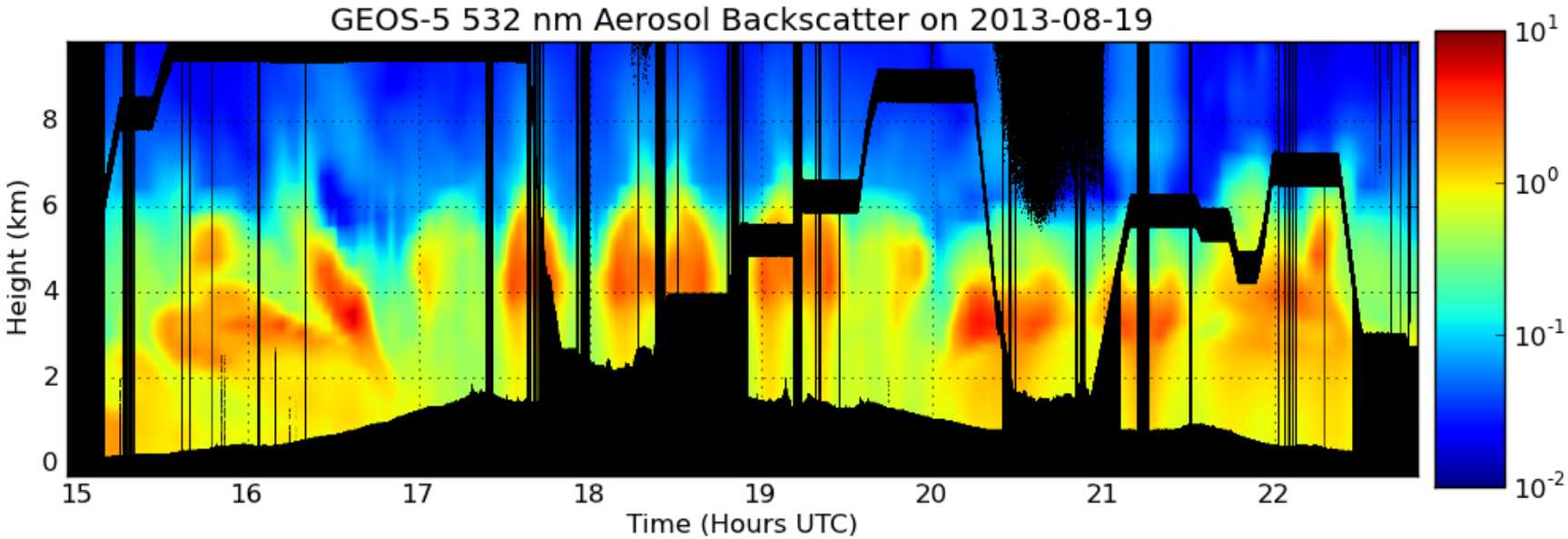
$$\chi = \nabla^{-2}\left[(\overline{E} + \overline{P} - \overline{L} + \frac{\overline{\langle \Delta q^a \rangle}}{\tau}\right]$$

Data Assimilation and Field Campaigns

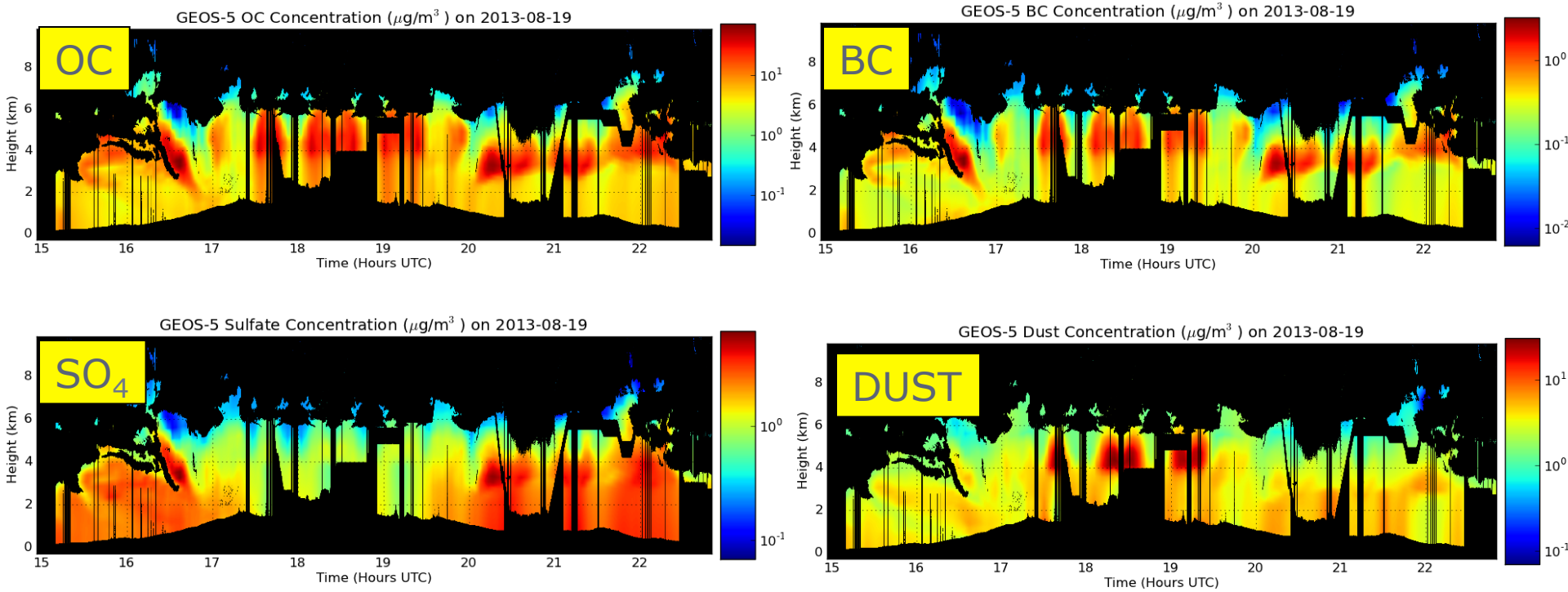
- Assimilation of localized field campaign data in a global model is of limited utility
  - Impact is often downstream of measurement
- However, field campaign data provide a great opportunity for DA algorithm development
  - Produce analysis along a flight curtain
  - Use model state sampled at curtain as prior
  - Include measurements from multiple sensors polarimeters, radiometers, LIDAR
  - Update model state, verify against in-situ payload

HSRL/Dial & GEOS-5 During SEAC4RS



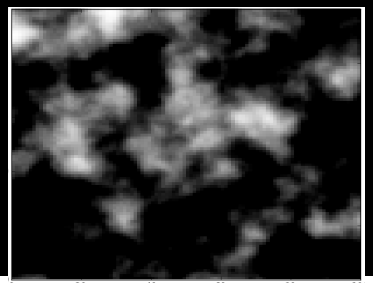


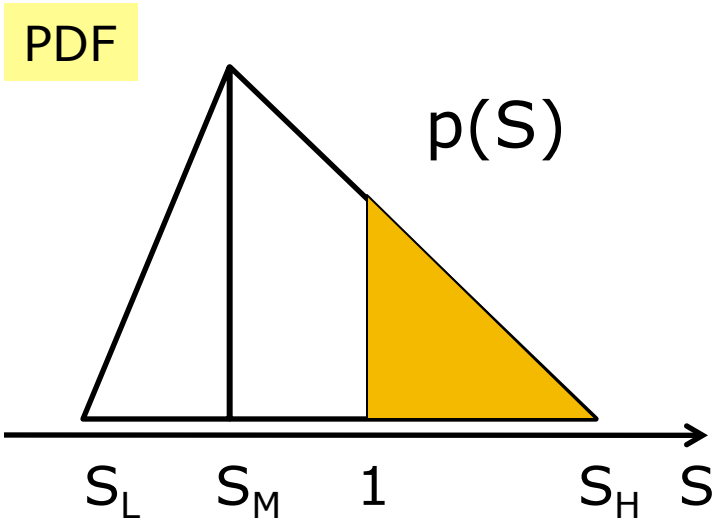
GEOS-5 Species: Background



Except for Dust, all particles assumed spherical

Clouds & Sub-grid Variability





$$S = (q_v + q_L + q_I) / q_S(T)$$

- PDF-based cloud parameterizations provide very useful information about sub-grid variability
- Given a PDF of total water one can generate sub-columns consistent with that PDF
- Observation simulators can account for representativeness error by operating on these sub-columns

Bayesian Parameter Estimation

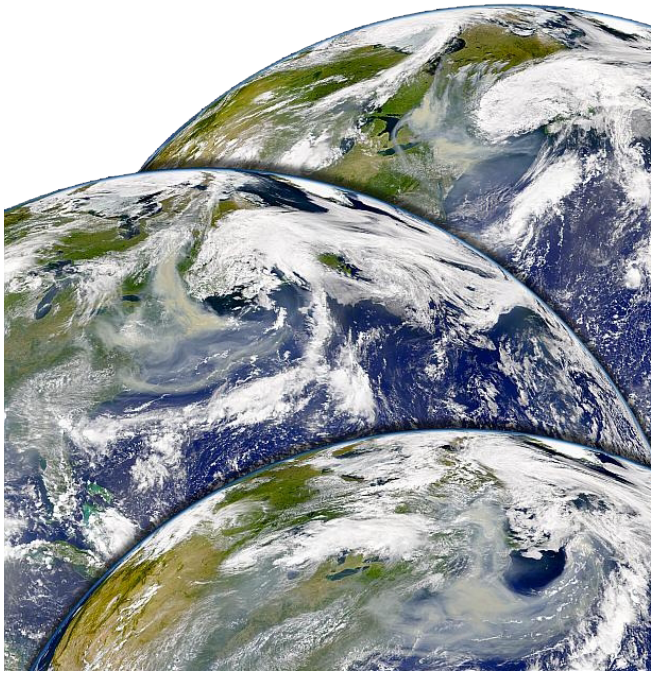
- Within a grid column, consider a set of measurements

$$\boldsymbol{y} = (y_1,\ldots,y_P)$$

  say MODIS cloud top pressure, cloud optical depth
- Goal:
  - estimate PDF parameters α_k
  - Given the observations $\boldsymbol{y}$
- Bayes theorem:

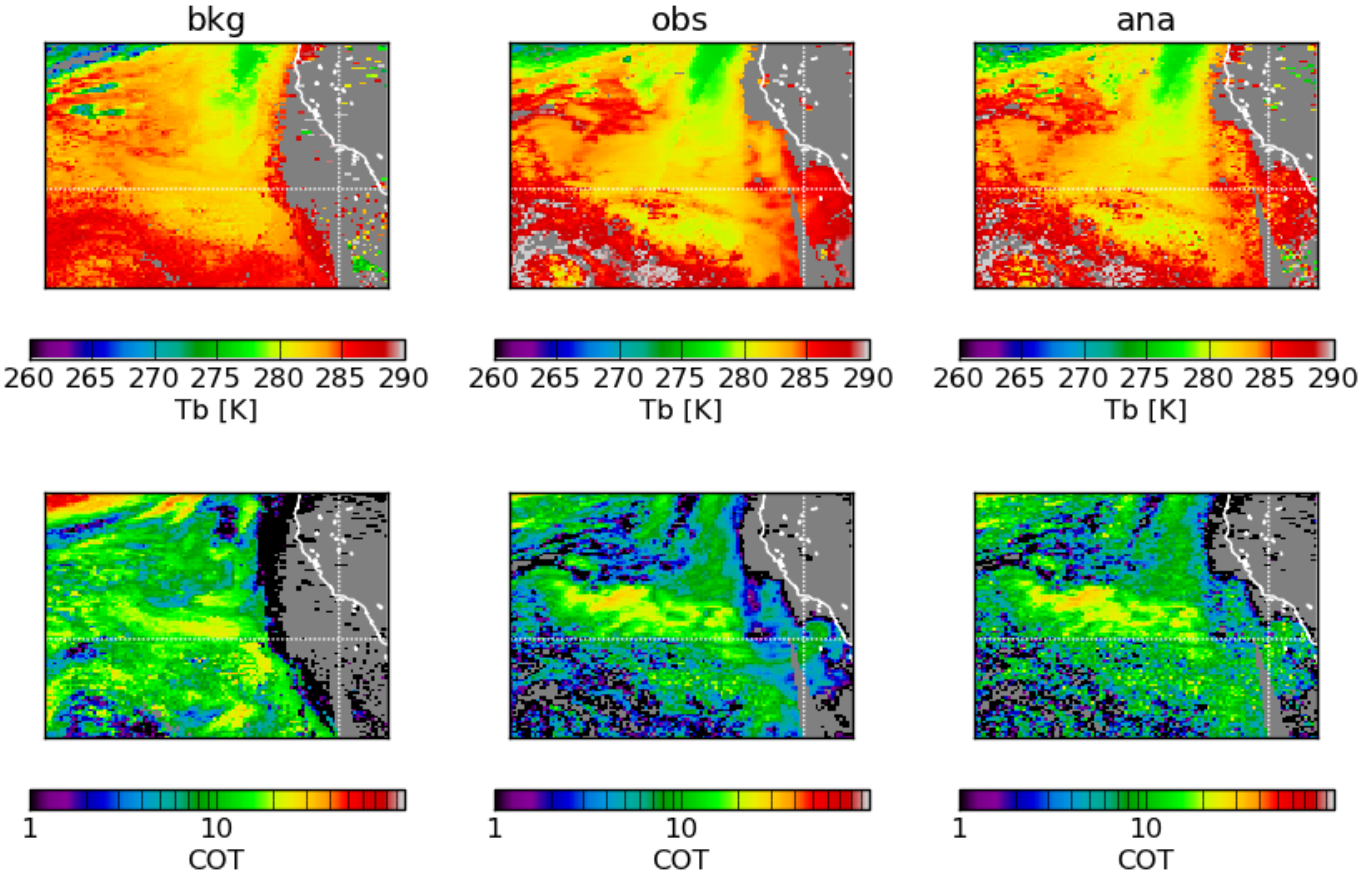
$$p(\alpha|\boldsymbol{y}) \sim p(\boldsymbol{y}|\alpha)\, p(\alpha)$$

- Maximum-likelihood estimation
  - Find α that maximizes $p(\alpha|\boldsymbol{y})$
- In short: find PDF parameters that "matches" MODIS hi-res data



Markov Chain Monte Carlo Method

Stratocumulus



O.S.S.E.

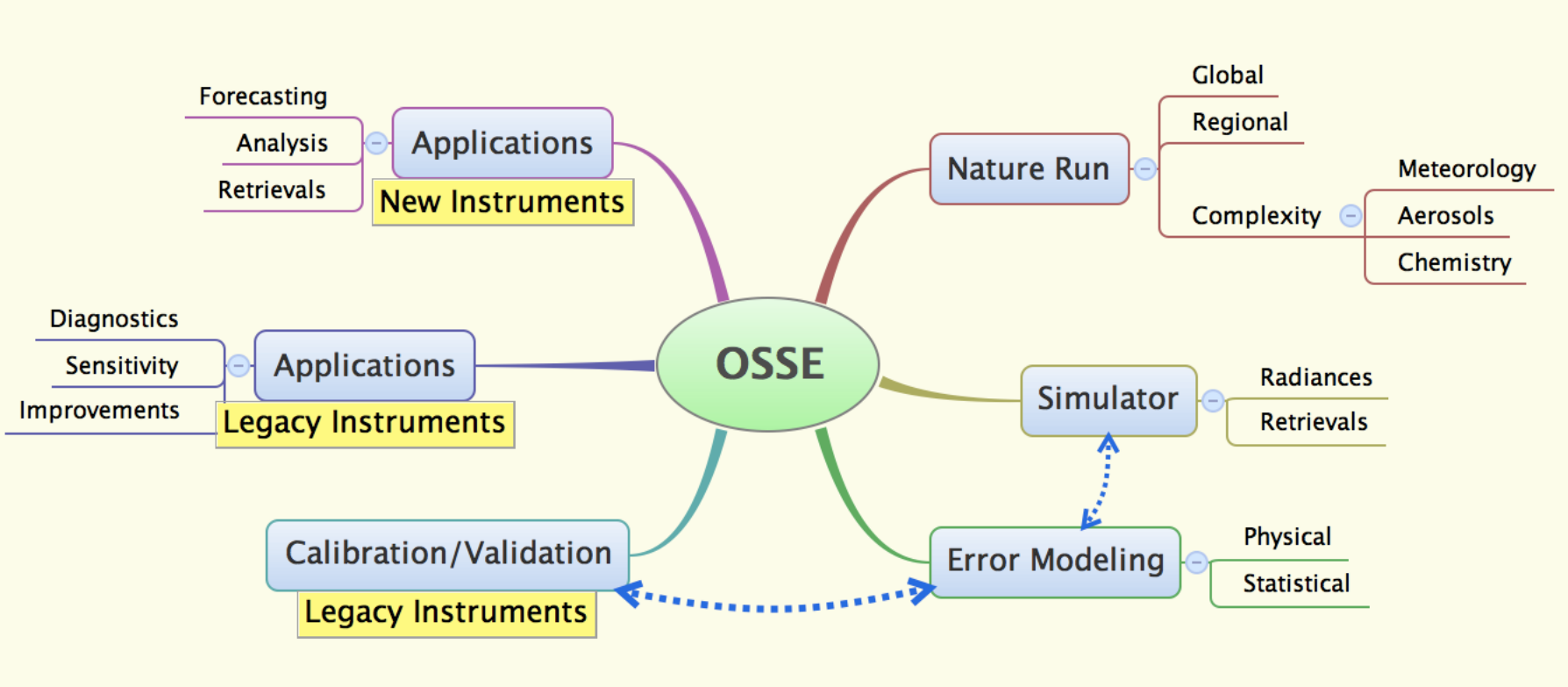
- Observing System
- Simulation
- Experiment

Model-based OSSE

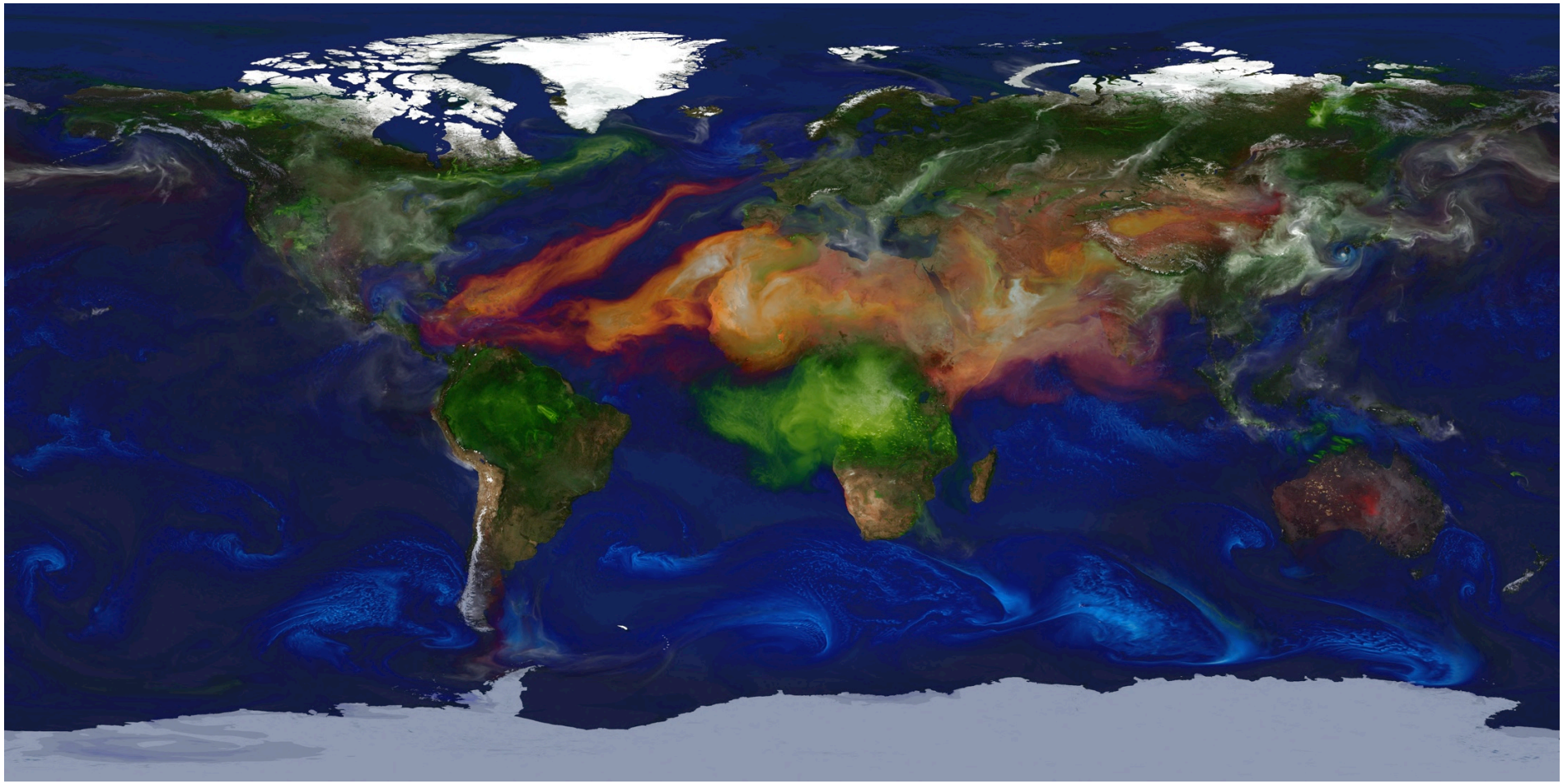
A framework for numerical experimentation in which *observables* are simulated from fields generated by an earth system model, including a *parameterized* description of the *observational error* characteristics.

Simulations are performed in support of an experimental goal.

Elements of an OSSE System

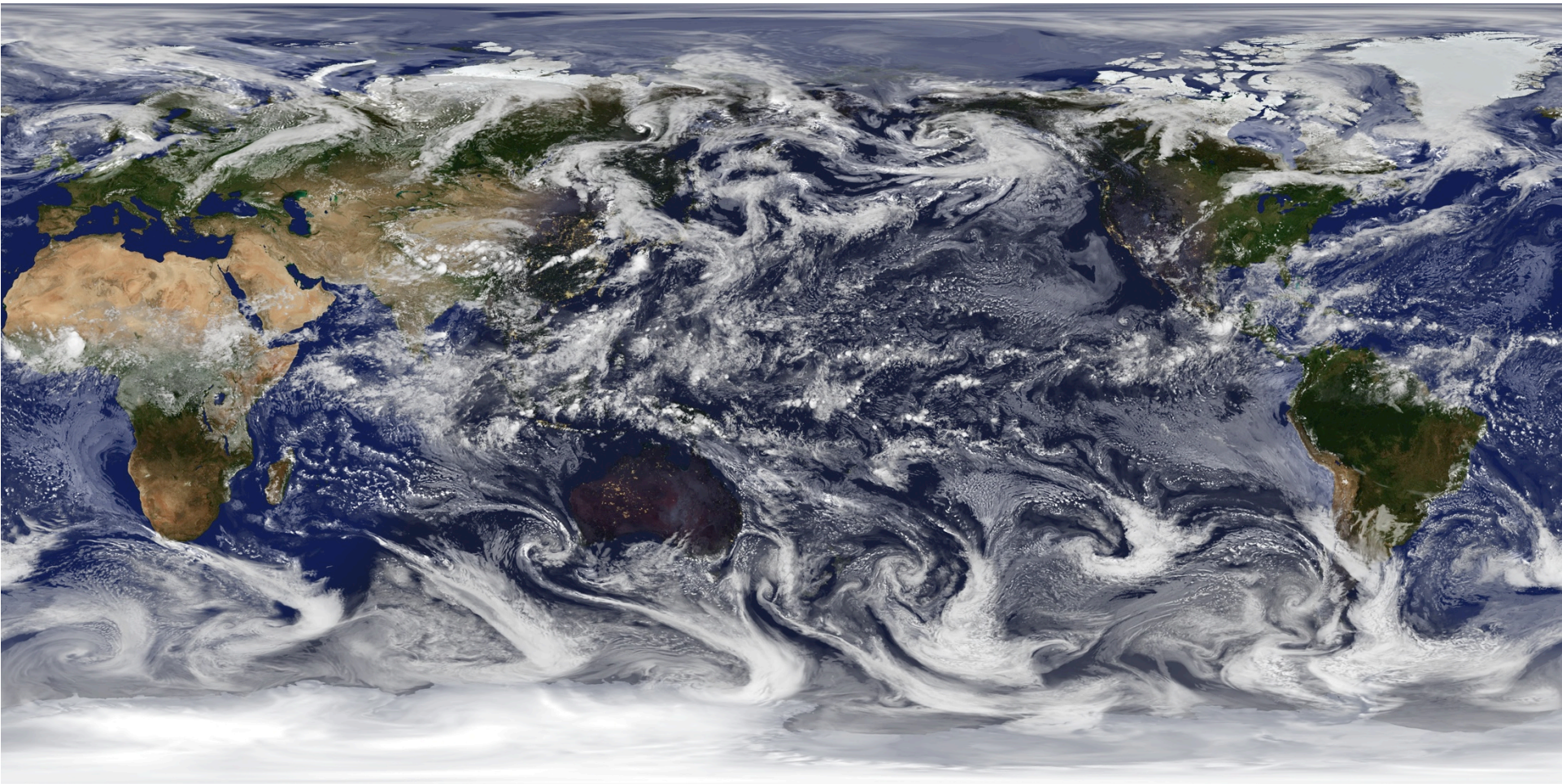


GEOS-5 Nature Run: Aerosols



GEOS-5 Non-hydrostatic 7 km Global Mesoscale Simulation

GEOS-5 Nature Run: Clouds



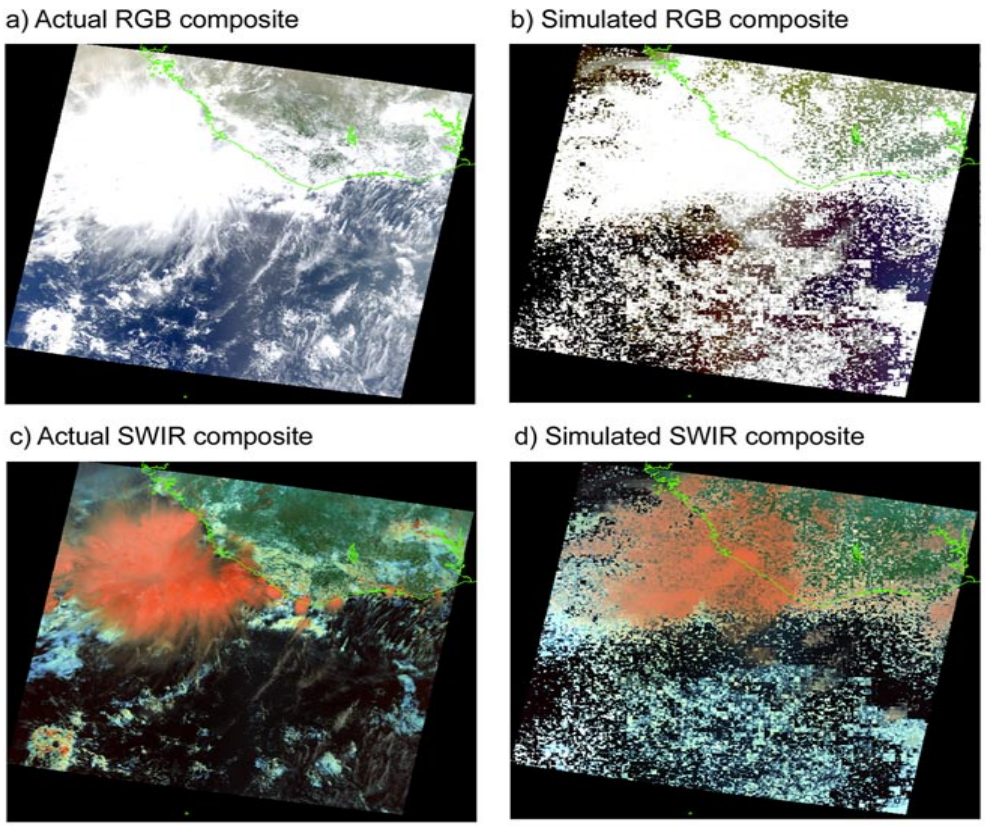
GEOS-5 Non-hydrostatic 7 km Global Mesoscale Simulation

OSSE: Types of Simulators

- Level 1 simulators
  - Detailed radiative transfer calculation in the presence of clouds, aerosols, ice, etc.
  - Instrument characteristics
  - Observables: polarized radiances, backscatter
- Level 2 simulators
  - Retrieved quantities at observation location
  - Averaging kernels, error characteristics
- Level 3 simulators
  - Hourly to seasonal mean statistics sampled at the instrument footprint

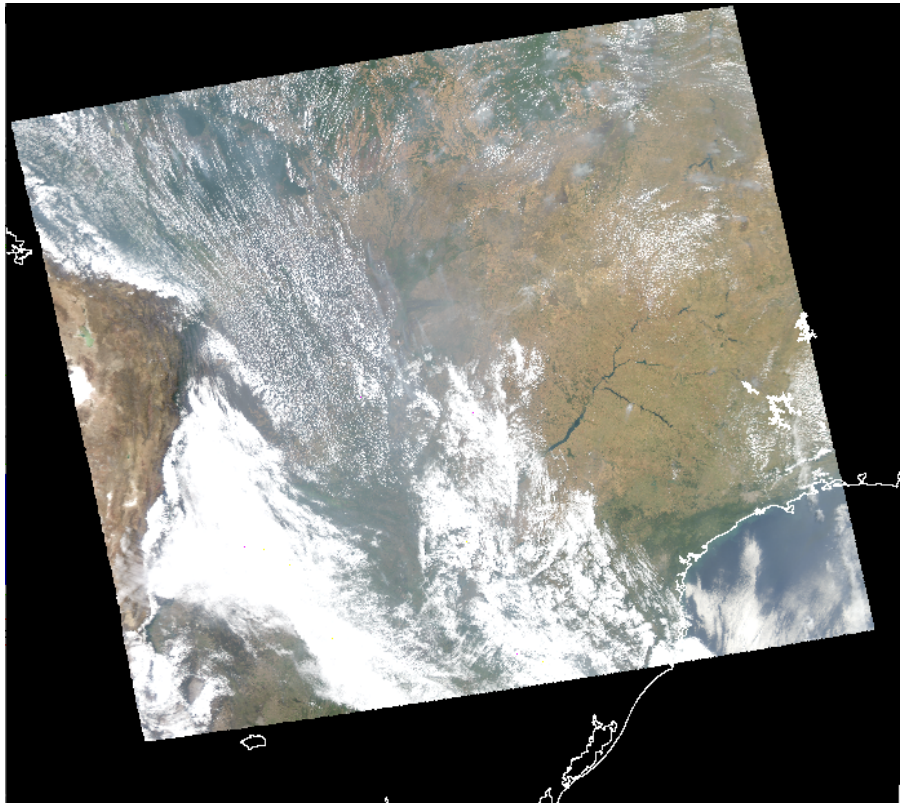
MODIS Cloud & Aerosol Retrieval Simulator

- PDF based sub-grid sampling of GEOS-5 fields (ICA)
- Spatial "clumping"
- Radiances for 27 MODIS channels
- Cloud and aerosol extinction, ssa, phase function
- Operational Retrievals
  - Clouds: MOD06
  - Aerosols: MOD04

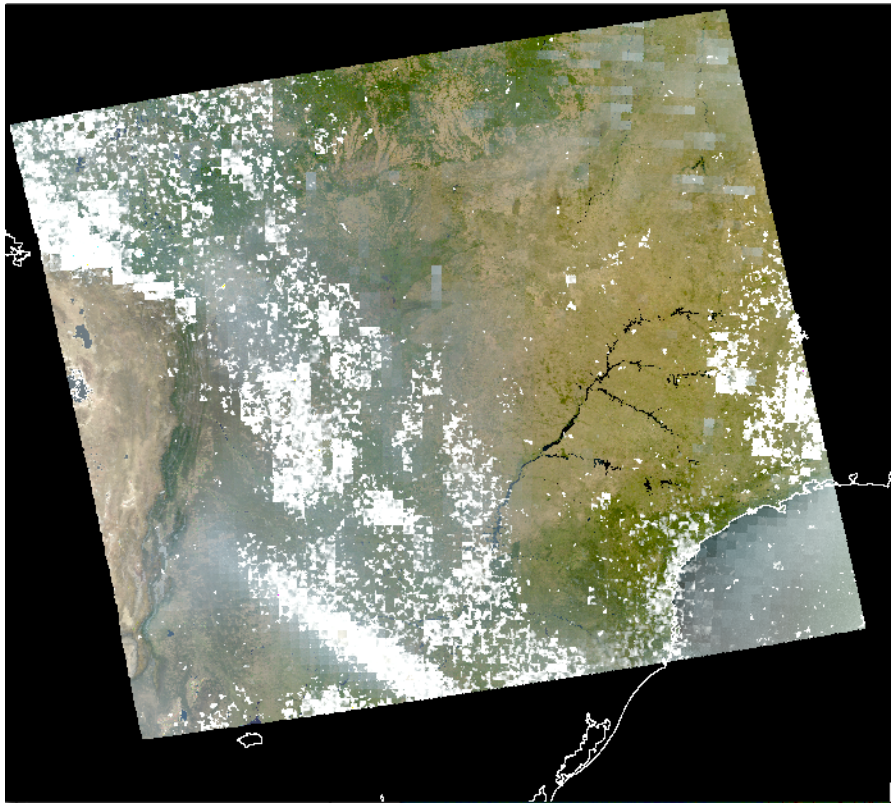


Wind et al., 2013, GMD

MODIS Level 1 Simulator



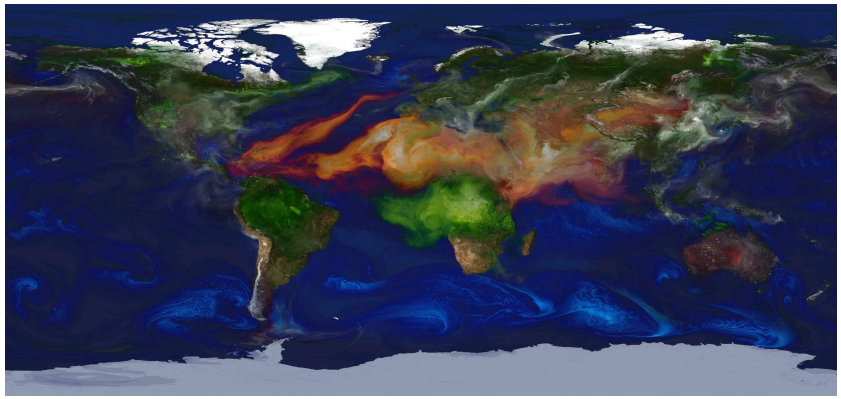
MODIS Aqua

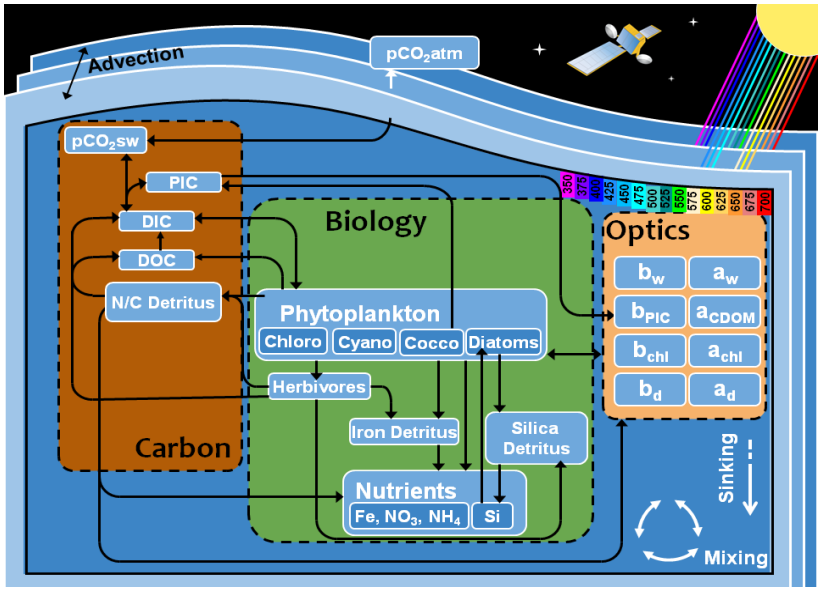


GEOS-5 25 km Simulation

PACE Simulator

- GEOS-5 non-hydrostatic 7 km atmosphere with GOCART aerosols
- Coupled to GEOS-5 10 km ocean component with biogeochemistry
- Simulation of
  - Water leaving radiances
  - t.o.a. reflectances





Summary: Data Assimilation for ACE

- **Flight Path 2D-Var:**
  - Control variable:
    - Model Prognostic State
  - Prior:
    - Model as background
  - Observations
    - LIDAR
    - Polarimeters
    - Radiometers
  - Validation
    - In-situ measurements
- **OSSEs:**
  - Simulators: L1, L2, L3
  - Trade-off studies
  - Algorithm Development
    - Retrieval
    - Data assimilation
- **Post-Launch:**
  - Level 4 products
  - Level 2x for monitoring
  - Complete re-analysis (IESA)