National Aeronautics and Space Administration

Aerosol and Trace Gas OSSE Capabilities at Goddard

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CEOS Atmospheric Composition Virtual Constellations

College Park, Maryland

4 May 2018

Outline

- Introductory Remarks
- GEOS Nature Run Update
- OSSE Studies Highlights
- Overview of other A&RG OSSE activities
- Concluding Remarks

Carbon cycle related OSSEs covered in Lesley Ott's Talk

O.S.S.E.

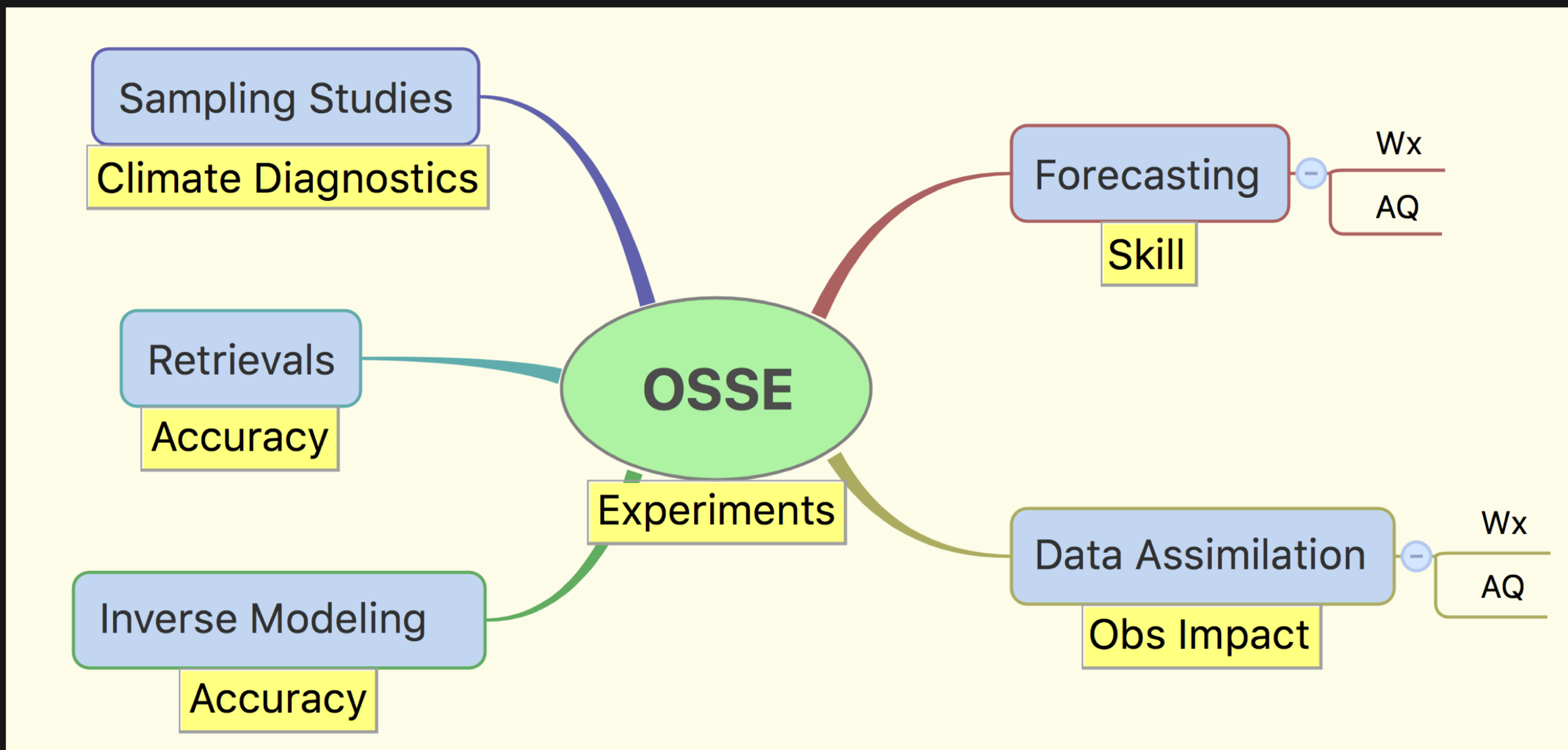
- Observing System
- Simulation
- Experiment

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.

The “E” in OSSE

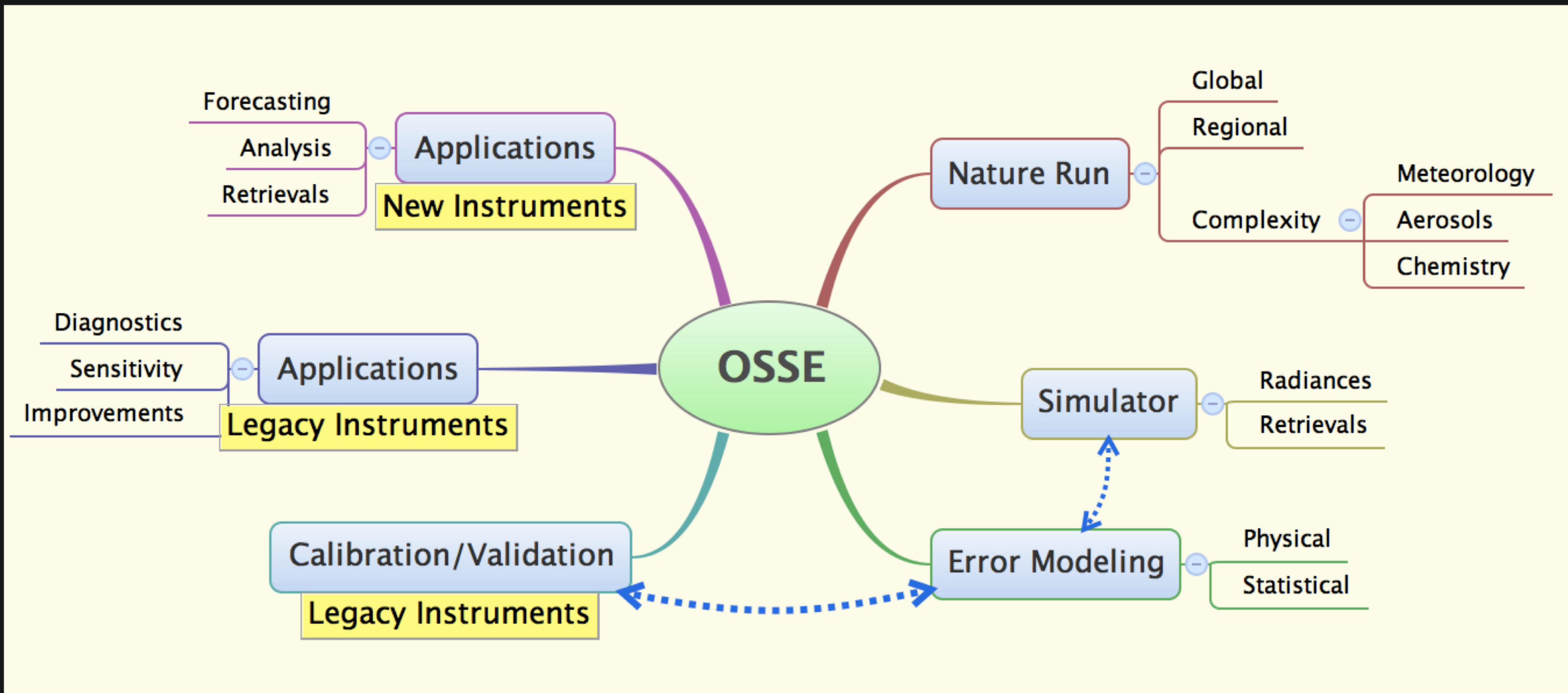

Sampling Studies
Climate Diagnostics
Retrievals
Accuracy
Inverse Modeling
Accuracy
OSSE
Experiments
Forecasting
Skill
Wx
AQ
Data Assimilation
Obs Impact
Wx
AQ

The Validation Imperative

- As with any simulation, OSSE results apply to new instruments only to the degree they have been validated with existing legacy instruments.
- OSSE credibility is first determined by carefully comparing a variety of statistics that can be computed in both the real and OSSE simulated contexts.

OSSEs need to be validated as a *System*

Elements of an OSSE System



GEOS Nature Runs

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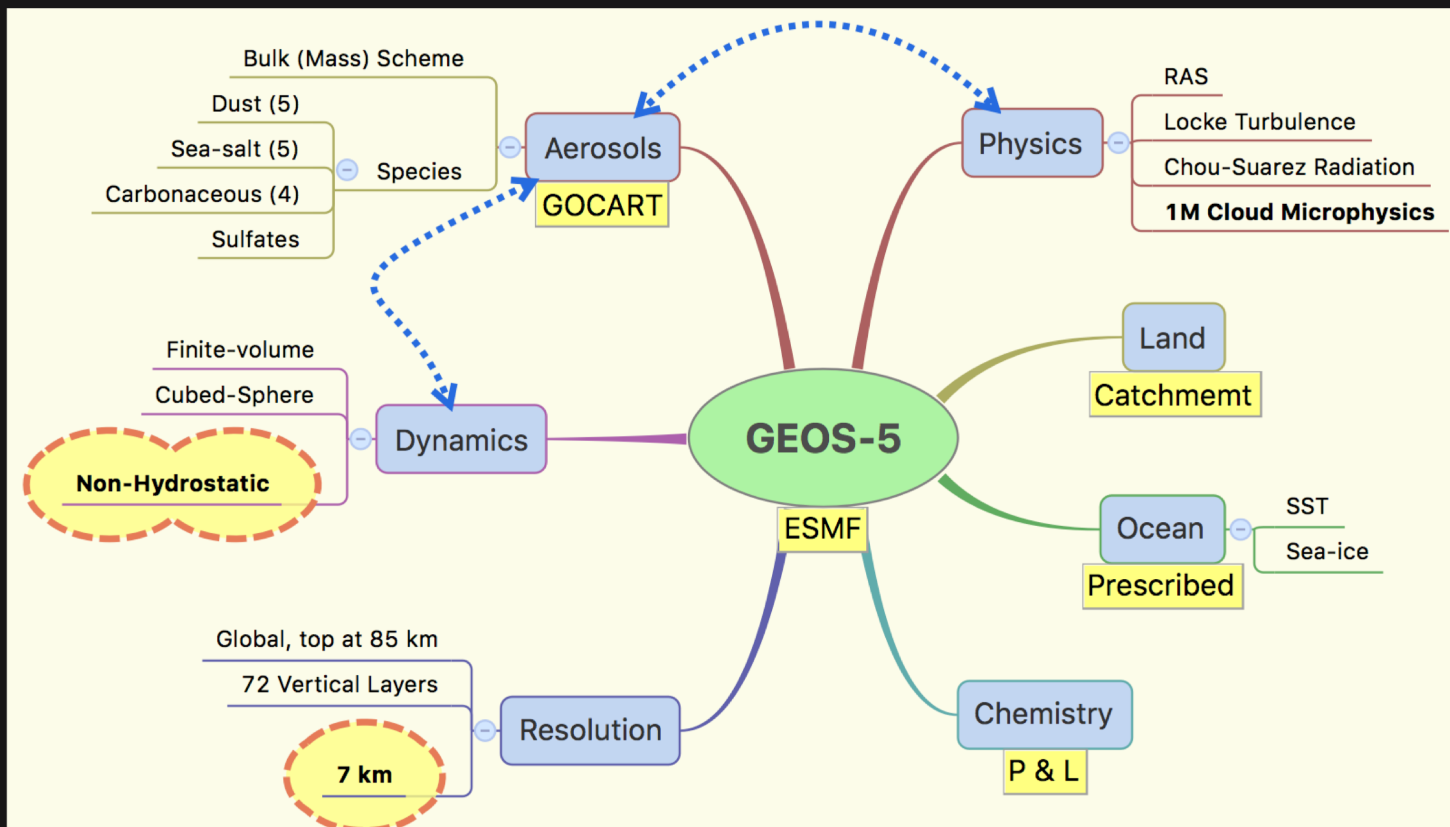
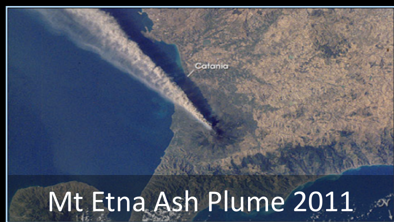
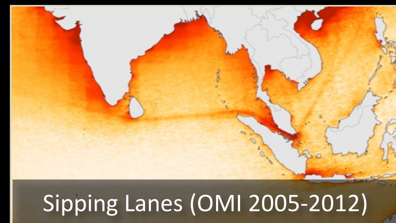
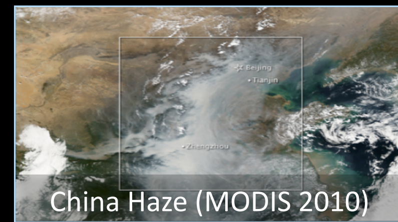
GEOS Global 7km Nature Run: 2 Years

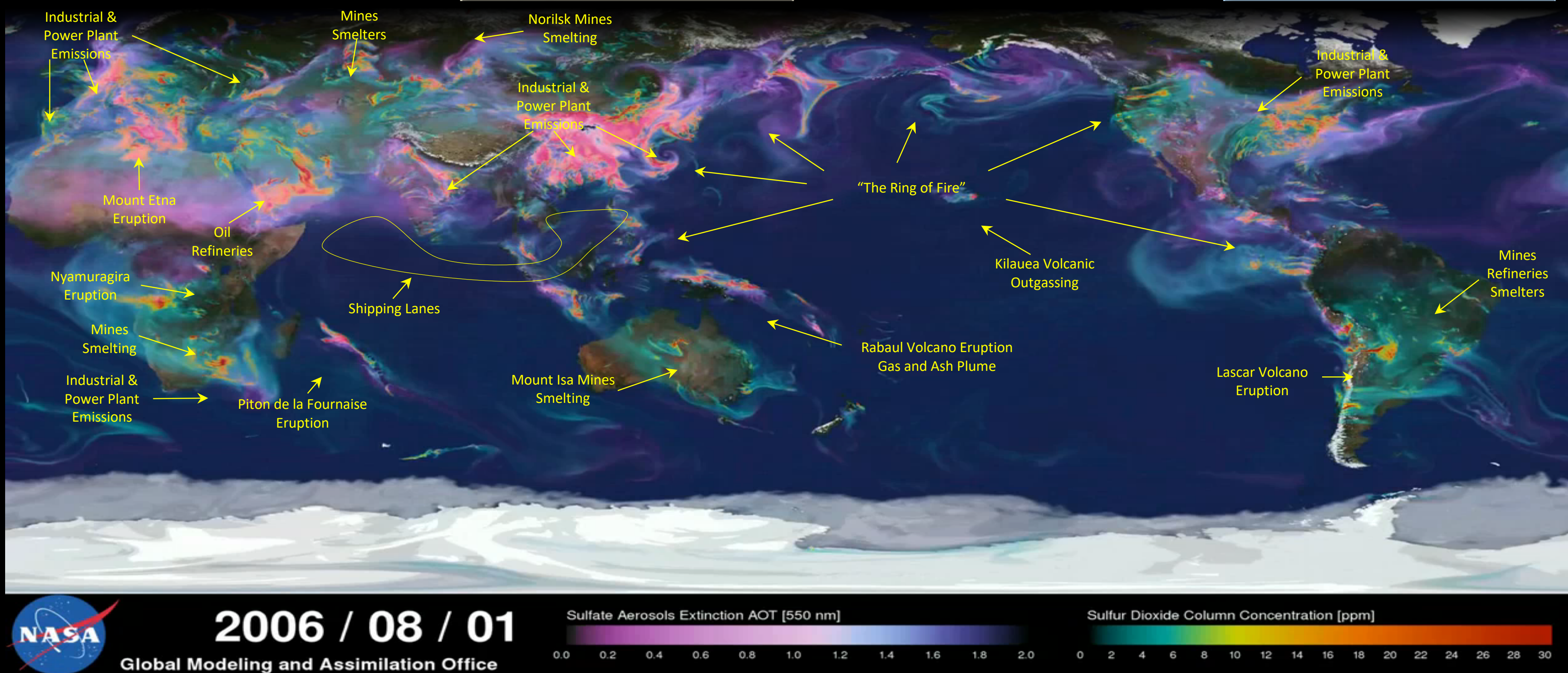


G5NR: Sulfate and Sulfur Dioxide





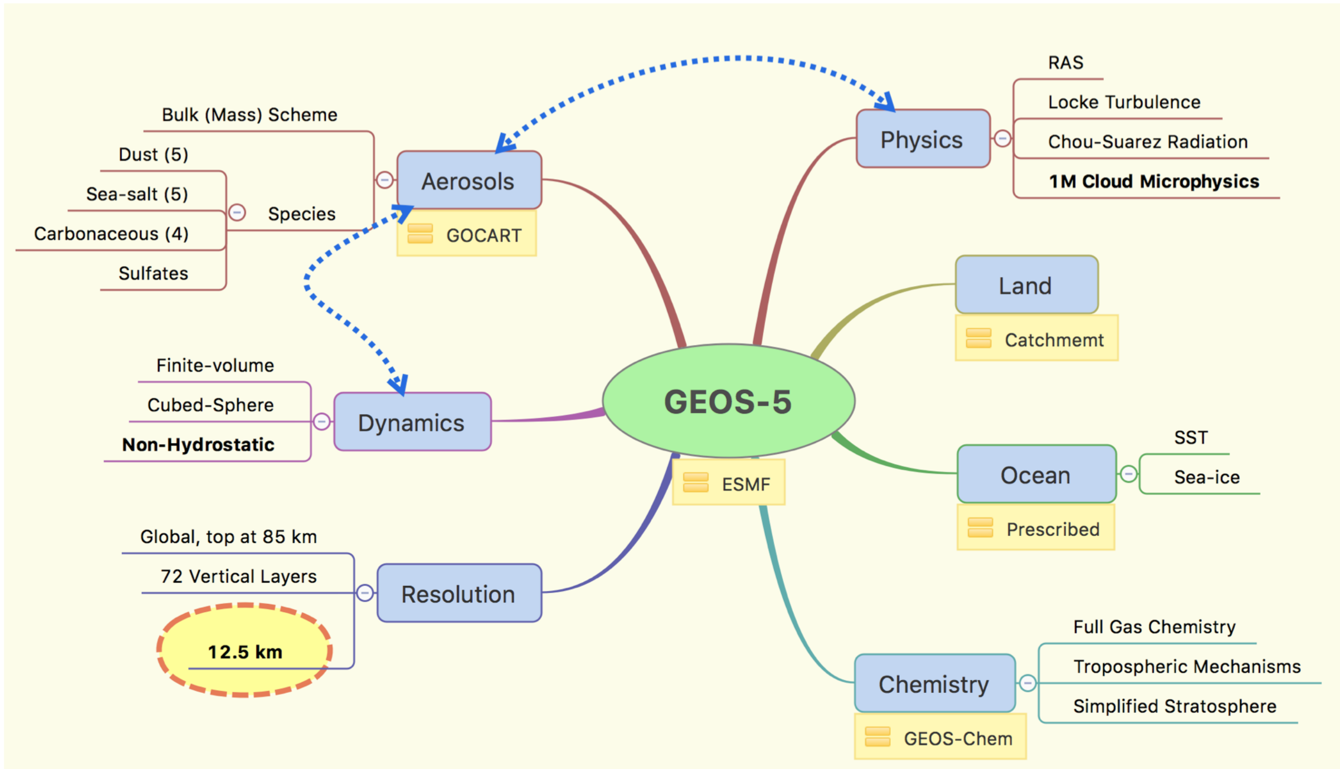




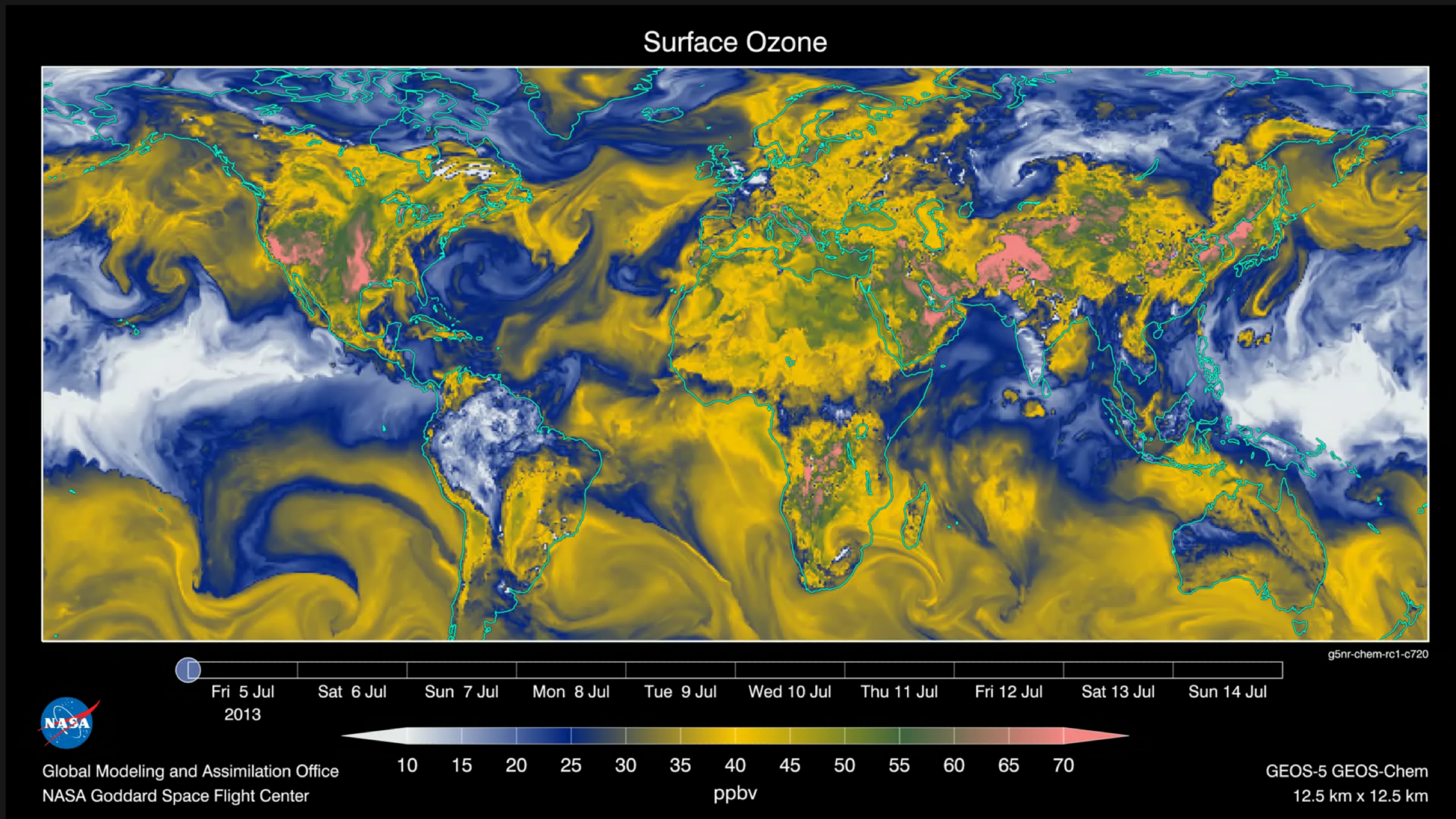
G5NR-Chem

GEOS-5 Nature Run with Full Gas Chemistry

- Period: July 2013-June 2014, May-June 2016
- Validation: **SEAC4RS, KORUS-AQ**
- Chemical mechanisms from GEOS-Chem, simplified statrosphere
- Meteorology constrained by MERRA-2 downscaling
- Hourly output of 3D *retrievable gases*
- Documentation in prep:
  - File Spec
  - Model Configuration
  - Evaluation Tech Memo



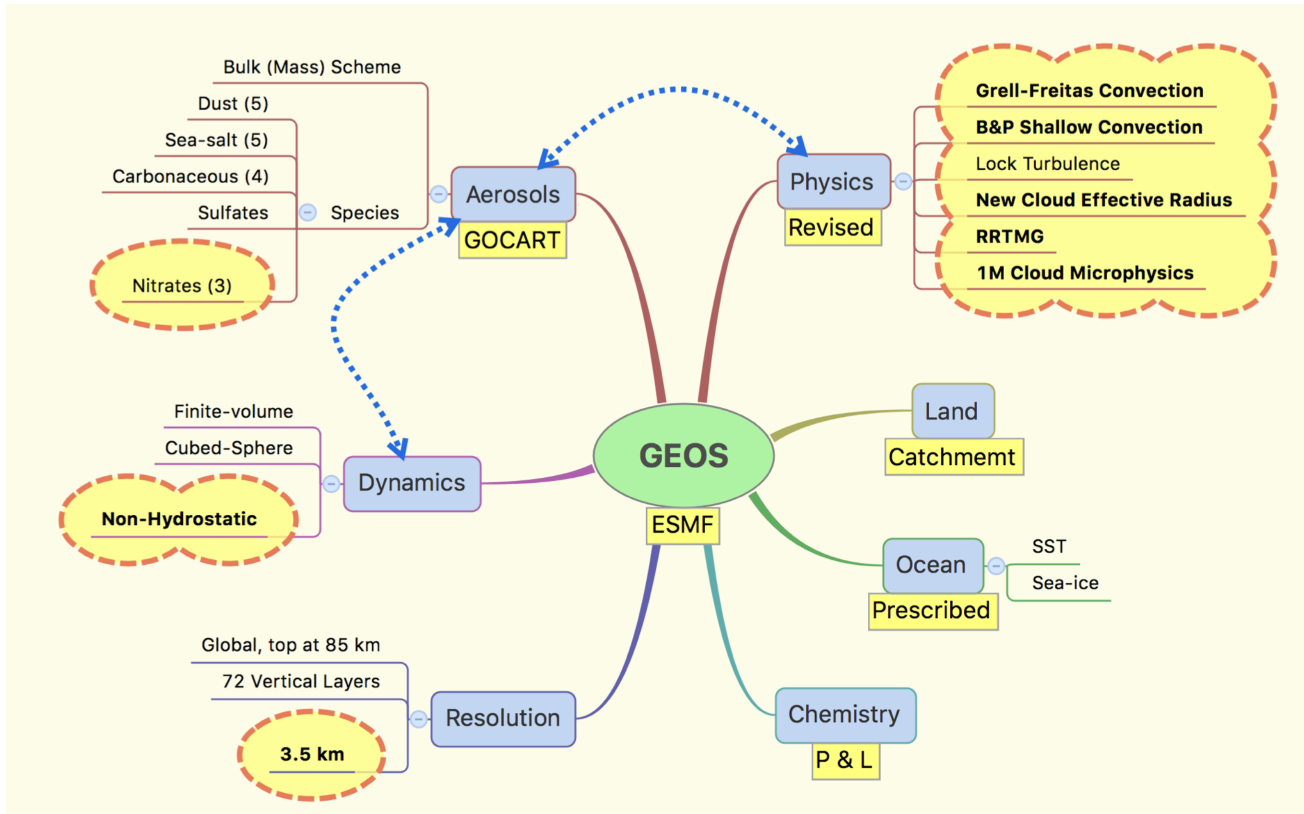
Surface Ozone



Coming Soon

3.5 km GEOS Nature Run with Interactive Aerosols

- Period: **August 2016**
- Validation: **ORACLES**
- Revised model physics
- Direct and Indirect Aerosol Effect
- Meteorology constrained by GEOS-FP downscaling
- *Full G5NR output suite*
- Model undergoing final tuning
- Expected completion:
    - **Fall 2018**



OSSE Activities

Highlights

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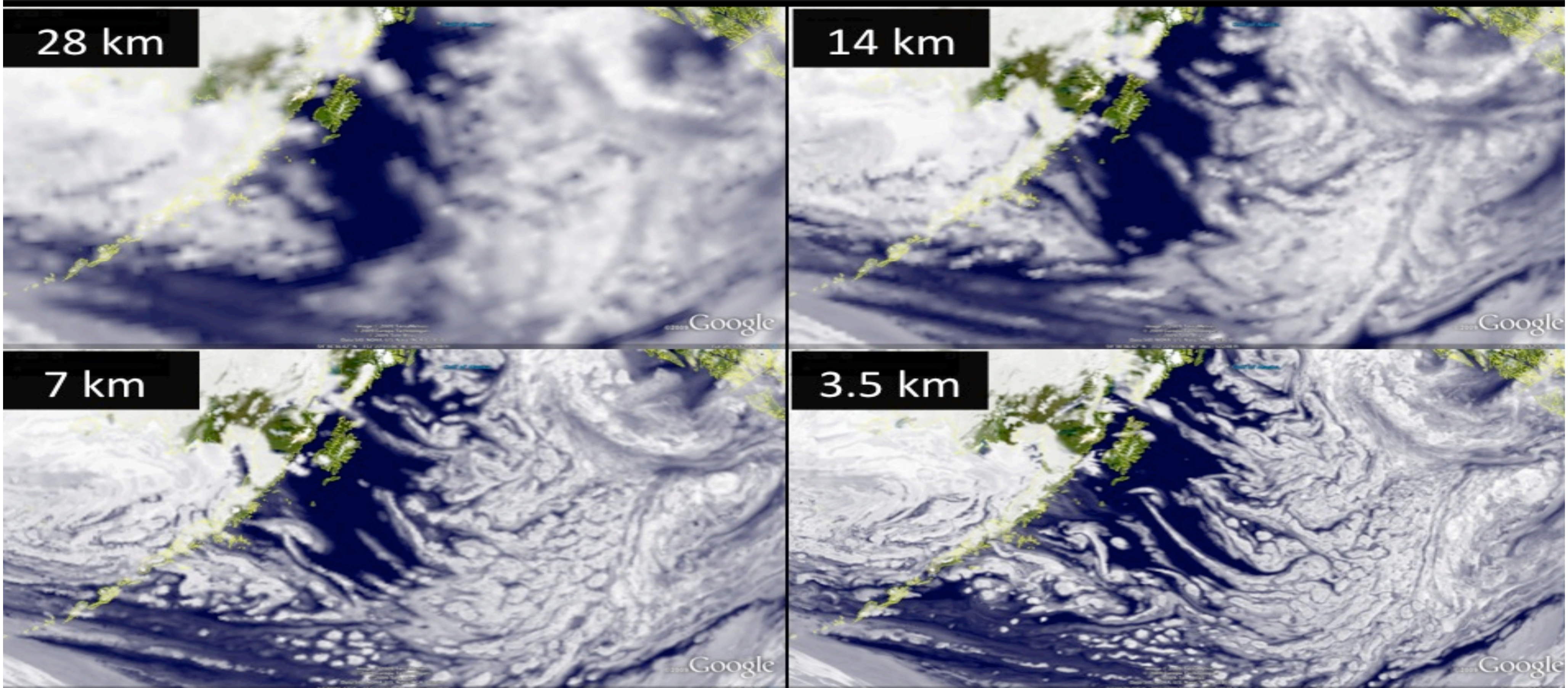
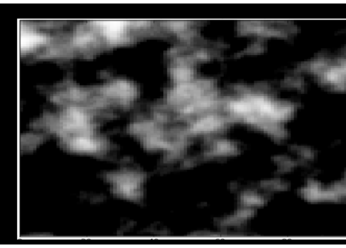
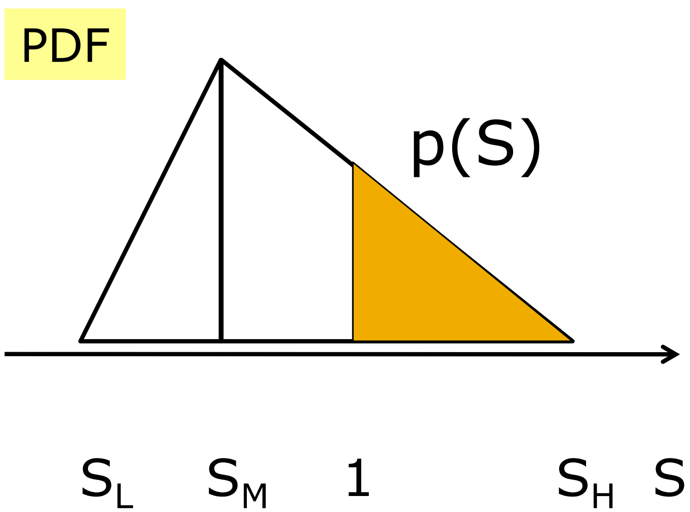
Sub-grid Variability



Clouds & Sub-grid Variability





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

Norris and da Silva, 2016

- 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

MODIS Cloud & Aerosol Retrieval Simulator

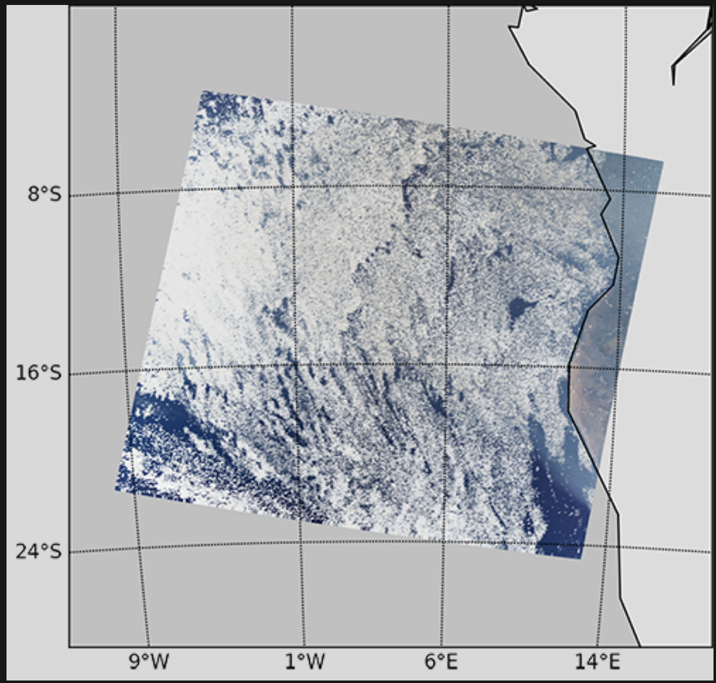
- Algorithm proofing sandbox
- 1km MODIS sensor geometry + 7km GEOS-5 Nature Run + Total Water PDF sampling to go from 7km to 1km
- 25 MODIS channels (410nm – 14.2μm)
- Correlated-k atmospheric transmittance model
- DISORT-5 radiative transfer core
- Output to standard 1-km MODIS radiance file

- Any data product code runs as if presented with real data, no awareness of radiance source
- Can examine retrieval code in fine detail
- HPC application (400 processors, 8.5 hours wall-clock-time, 32 streams per granule)

Wind et al. 2013, 2016.

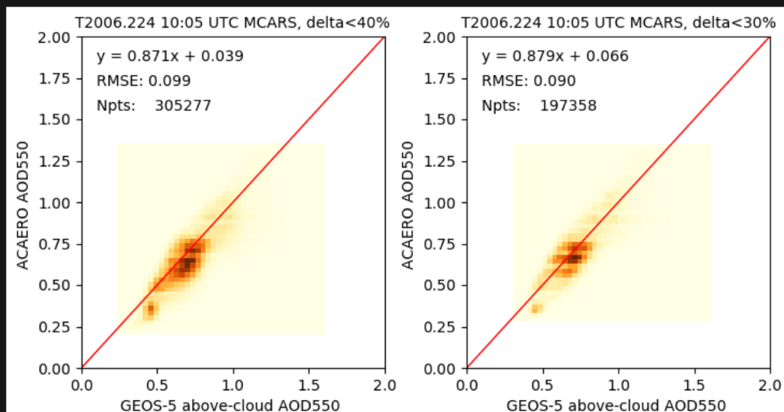
MODIS ACAERO Algorithm Evaluation

- MODIS Above-Cloud Aerosol Optical Properties by K. Meyer
- Returns aerosol optical depth, cloud optical thickness and cloud effective radius with pixel-level uncertainty at 1km resolution
- Uses 6 MODIS channels (440nm – 2.1μm)
- MODIS Dark-Target operational absorbing aerosol model
- Above-cloud retrievals over marine boundary layer clouds
- Uses MODIS Cloud product for cloud top pressure and cloud thermodynamic phase information
- Ran during ORACLES campaign as a near-real-time (NRT) product

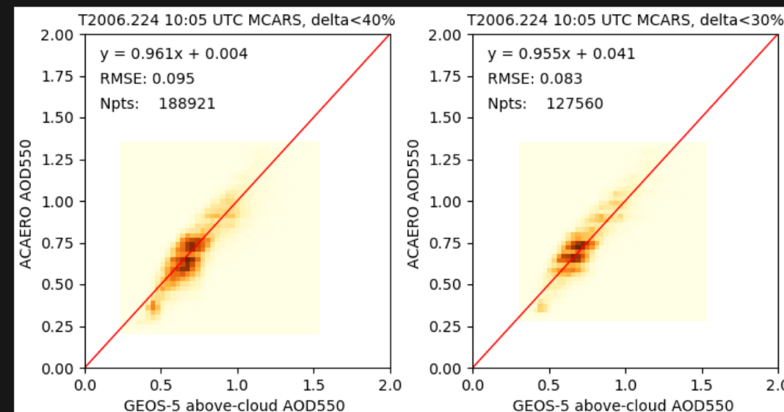


Wind et al. 2018, *in preparation*.

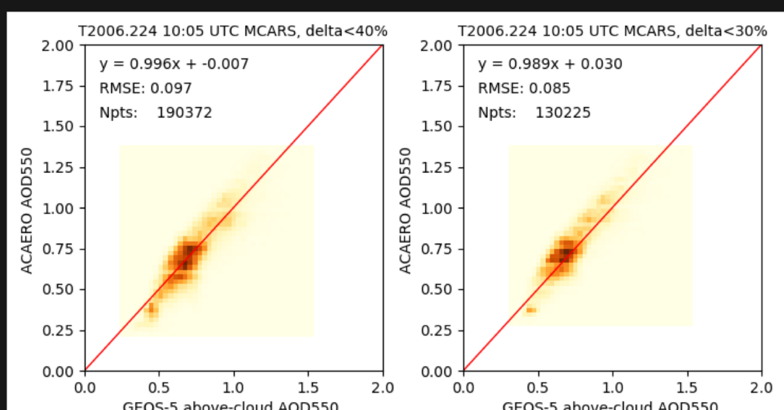
Add screening by sensor zenith < 30 degrees



by sensor zenith < 20 degrees



Add GEOS-5 input as ancillary



Recipe

Assimilate points with:

1. Pixel-level uncertainty < 40%
2. Cloud optical thickness > 4
3. Avoid the rainbow scattering angle
4. Select pixels with sensor zenith < 20°

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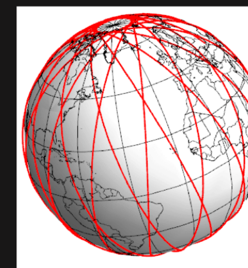
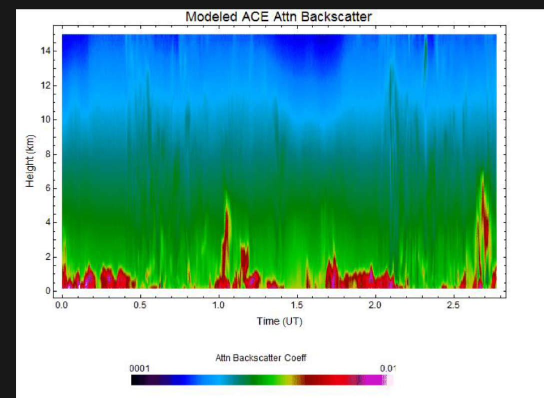
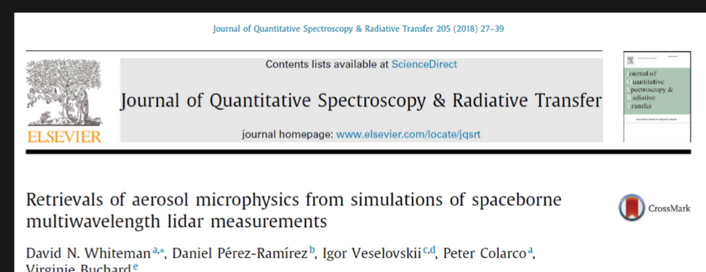
ACE Lidar Simulator

- GEOS provides a consistent set of optical and aerosol micro-physical data to use as input to lidar model and as reference for inversions
- Simulate HSRL lidar measurements for 24-hr Calipso orbit July 15, 2009 at 10 s resolution
  - 8640 density and 3β+2α aerosol optical profiles from GEOS-5
  - Radiance values from RT model (VLIDORT)
- Study yields for microphysical retrievals considering both 3β+2α and 3β+1α configurations
- Study microphysical inversions using original GEOS-5 optical data and simulated lidar data. Compare with GEOS-5 references.



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journal homepage: www.elsevier.com/locate/jqsrt

ELSEVIER

Retrievals of aerosol microphysics from simulations of spaceborne multiwavelength lidar measurements

David N. Whiteman[a,*], Daniel Pérez-Ramírez[b], Igor Veselovskii[c,d], Peter Colarco[a], Virginie Buchard[e]

RMS Difference Between GEOS-5 Microphysics and LIDAR Inversions

Case A: η > 0.75 (Fine Mode Predominance)

	Errors 0-15 %				Errors 15-20 %				Errors 20-30 %				Errors 30-40 %				Errors 40-50 %			
	Reg.	Reg. 3b1a 532	LE	LE 3b1a 532	Reg.	Reg. 3b1a 532	LE	LE 3b1a 532	Reg.	Reg. 3b1a 532	LE	LE 3b1a 532	Reg.	Reg. 3b1a 532	LE	LE 3b1a 532	Reg.	Reg. 3b1a 532	LE	LE 3b1a 532
R_{eff}	48.6	59.3	44.9	73.3	51.2	53.2	45.6	64.9	54.4	55.2	49.7	67.2	53.2	56.4	47.3	68.3	48.9	59.8	43.1	61.2
V	16.2	18.4	22.1	30.5	16.7	17.7	21.5	28.4	19.6	19.4	23.5	28.4	17.7	17.6	21.2	26.2	16.5	17.3	20.1	25.3
S	34.3	39.3	35.3	52.3	33.7	37.3	35.0	49.3	37.0	38.7	34.5	48.9	35.5	37.0	32.0	47.2	36.0	35.9	28.2	43.4
m_r	0.03	0.03	0.04	0.03	0.03	0.03	0.04	0.03	0.04	0.03	0.04	0.03	0.04	0.03	0.04	0.03	0.04	0.04	0.05	0.03
m_i	9E-3	8E-3	8E-3	8E-3	8E-3	8E-3	8E-3	7E-3	8E-3	8E-3	7E-3	7E-3	8E-3	8E-3	8E-3	8E-3	7E-3	7E-3	7E-3	7E-3

Case B: 0.25 < η < 0.75 (Mixture)

	Errors 0-15 %				Errors 15-20 %				Errors 20-30 %				Errors 30-40 %				Errors 40-50 %			
	Reg.	Reg. 3b1a 532	LE	LE 3b1a 532	Reg.	Reg. 3b1a 532	LE	LE 3b1a 532	Reg.	Reg. 3b1a 532	LE	LE 3b1a 532	Reg.	Reg. 3b1a 532	LE	LE 3b1a 532	Reg.	Reg. 3b1a 532	LE	LE 3b1a 532
R_{eff}	40.5	22.6	52.1	23.0	42.4	24.4	52.3	24.8	44.4	24.2	54.2	25.6	52.0	28.2	58.2	25.4	52.1	33.1	57.8	25.8
V	28.1	19.9	52.5	40.1	30.7	22.0	52.0	39.7	32.1	22.6	53.7	40.7	37.0	23.5	57.2	44.0	36.6	28.8	56.5	39.8
S	43.6	22.1	16.0	26.2	46.7	23.4	17.0	27.3	49.7	23.8	17.4	27.6	60.0	24.9	19.1	29.5	67.8	25.6	21.9	28.8
m_r	0.11	0.13	0.08	0.08	0.11	0.13	0.08	0.08	0.10	0.12	0.08	0.08	0.11	0.13	0.09	0.08	0.11	0.12	0.09	0.08
m_i	2E-3	2E-3	5E-3	4E-3	2E-3	2E-3	5E-3	4E-3	3E-3	2E-3	5E-3	4E-3	2E-3	2E-3	5E-3	4E-3	2E-3	2E-3	5E-3	4E-3

Case C: η < 0.25 (Coarse Mode Predominance)

	Errors 0-15 %				Errors 15-20 %				Errors 20-30 %				Errors 30-40 %				Errors 40-50 %			
	Reg.	Reg. 3b1a 532	LE	LE 3b1a 532	Reg.	Reg. 3b1a 532	LE	LE 3b1a 532	Reg.	Reg. 3b1a 532	LE	LE 3b1a 532	Reg.	Reg. 3b1a 532	LE	LE 3b1a 532	Reg.	Reg. 3b1a 532	LE	LE 3b1a 532
R_{eff}	58.2	65.6	70.0	68.4	59.2	65.8	70.2	68.1	55.9	64.8	70.3	69.2	55.3	65.1	70.8	70.2	49.1	67.6	70.9	72.1
V	60.7	68.3	71.7	71.8	61.2	67.2	71.5	71.2	57.6	67.5	71.3	72.5	56.7	69.3	72.5	74.7	50.9	72.1	71.1	77.5
S	14.7	21.8	14.4	17.8	14.9	20.2	14.0	16.3	15.2	21.1	14.9	17.7	12.5	21.3	13.1	19.0	12.0	22.1	11.5	20.5
m_r	0.14	0.15	0.11	0.11	0.14	0.15	0.11	0.11	0.15	0.15	0.11	0.11	0.15	0.15	0.11	0.12	0.12	0.23	0.12	0.22
m_i	4E-3	3E-3	3E-3	3E-3	4E-3	3E-3	4E-3	3E-3	4E-3	3E-3	4E-3	3E-3	5E-3	4E-3	4E-3	4E-3	5E-3	4E-3	4E-3	4E-3

Fine/Coarse separation done based on GEOS-5 optical data

Lidar-Polarimeter Simulator

- **Surface:**
  - MODIS RTLS bi-directional reflectance
  - BPDF from Maignan et al. (2009)
    - Polarized reflectance that is a function of IGBP land use and NDVI
    - Fits POLDER measurements, spectrally flat
  - Possible to add on GISS Cox-Munk surface reflectance for ocean scenes if there is interest
- **Atmosphere**
  - 7 km Global GEOS-5 Nature Run (GOCART)
  - Rayleigh scattering
  - Optical properties are RH dependent
- **Orbits, Angles, and Wavelengths are speciable, for example:**
  - CALIPSO, ISS, 425 km orbit, etc…
  - VZA: 3.66, 11., 18.33, 25.66, 33, 40.33, 47.66, 55.0
  - Wavelengths: 354, 388, 410, 440, 470, 550, 670, 865, 1020, 1650, 2130
  - Observables: intensity, DoLP
- **RTM: VLIDORT v2.7**
- **Test simulation files can be found here.**
  - https://portal.nccs.nasa.gov/datashare/G5NR/c1440_NR/OBS/POLAR_LIDAR/CALIPSO/

Other OSSE Activities of Relevance

- **GMAO has a full Meteorological OSSE capability**
- Several GEO-CAPE related activities (P. Castellanos)
  - G5NR-chem, a Nature Run with full tropospheric tropospheric chemistry
  - Radiance simulator for several golden days (aerosol channels):
    - ✓ GOES-R, GEMS, TEMPO, SENTINEL-4
    - ✓ Hyper spectral trace gas capability in development
  - CO and AOD (forecast) OSSEs (David Edwards, J. Barré – NCAR)
- OMI/OMPS related activities
  - OMI Aerosol Retrieval Simulator (V. Buchard, P. Colarco, S. Gassó, O. Torres)
  - OMI SO2 source estimation evaluation (F. Liu, J. Joiner)
  - OMPS volcanic SO_2 retrieval OSSEs (E. Hughes, N. Krotkov, P. Colarco)
- AERONET retrieval OSSEs
- GRASP-ACE: joint lidar-polarimeter Retrieval OSSEs (D. Ramirez, O. Duovik)

Concluding Remarks

- A *credible* OSSE system requires well validated modeling components:
  - Nature run
  - Physical simulation of measurements
  - Instrument characterization and error modeling
- However, it must be validated as a *System*, by exercising it with the existing legacy observing system.
- OSSE applications such as *Retrieval OSSEs and sampling studies are as relevant to ACE as the classical analysis and forecast skill metric*
- Aerosol and Reactive Gases OSSE activities at Goddard:
  - High-resolution Nature Runs with coupled chemistry & aerosols
  - Retrieval OSSEs for cloud and aerosols (LEO and GEO)
  - Inverse Modeling OSSEs, evaluation direct emission estimation algorithms
  - Developing infra-structure for trace-gases observation simulations from GEO constellation

Relevant URLs

Site	URL
GMAO Home Page	https://gmao.gsfc.nasa.gov/
Weather Analysis & Prediction	https://gmao.gsfc.nasa.gov/weather_prediction/
GEOS NRT Product Information	https://gmao.gsfc.nasa.gov/GMAO_products/NRT_products.php
GEOS-FP File Specification	https://gmao.gsfc.nasa.gov/products/documents/GEOS_5_FP_File_Specification_ON4v1_1.pdf
GMAO Publications	https://gmao.gsfc.nasa.gov/pubs/
MERRA-2 Project Page	https://gmao.gsfc.nasa.gov/reanalysis/MERRA-2/
Forecast Web Visualizations	https://fluid.nccs.nasa.gov/weather/
GEOS 7km Nature Run (G5NR)	https://gmao.gsfc.nasa.gov/global_mesoscale/7km-G5NR/
G5NR-Chem Nature Run	https://portal.nccs.nasa.gov/datashare/G5NR-Chem/Heracles/12.5km/DATA/