



Simulated Proxy Data for PACE OCI Ocean Color and Aerosol Retrieval Algorithm Development

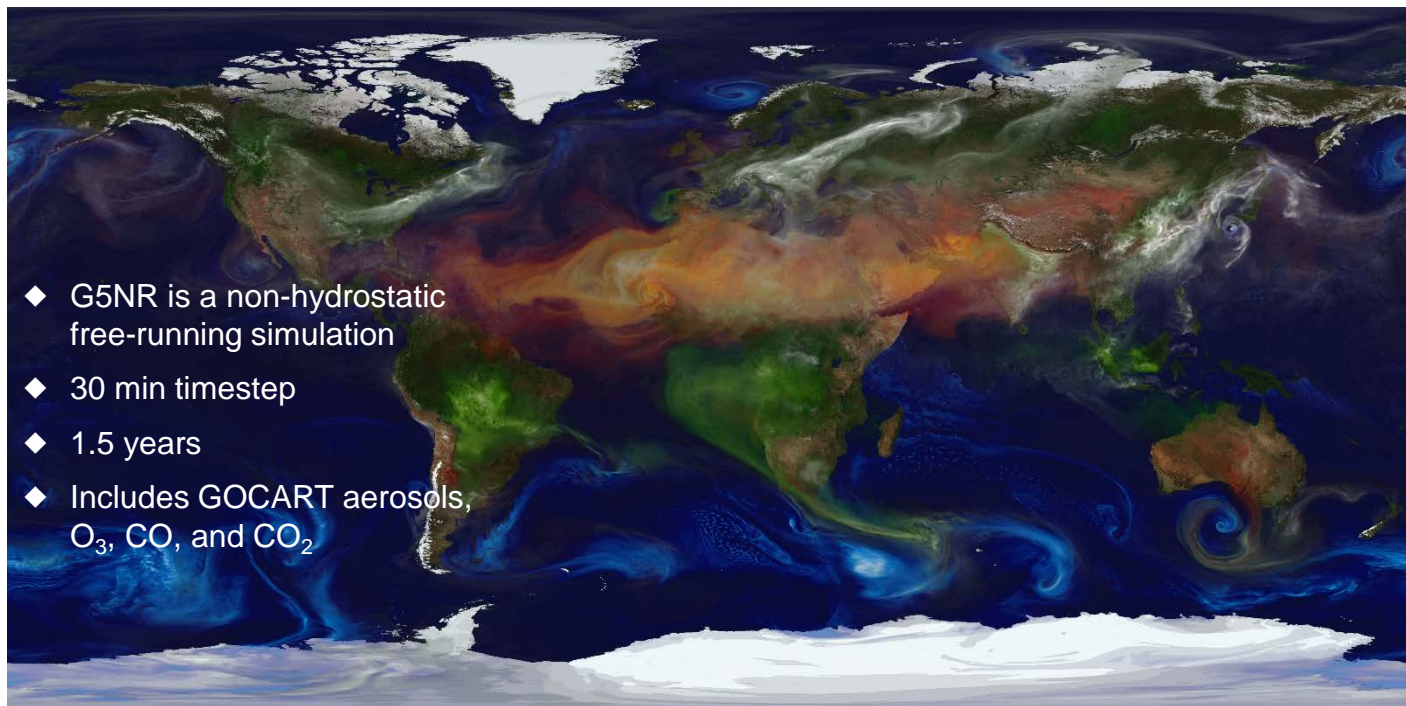
Patricia Castellanos

Amir Ibrahim (616), Andy Sayer (616), Samuel Anderson (616), Cecile Rousseaux (610.1),
Watson Gregg (610.1), Bryan Frantz (616), Jeremy Werdell (616), Arlindo da Silva (610.1),
Peter Norris (610.1), Robert Spurr (RT Solutions Inc.), PACE SDS Team

GMAO Developments to Support Observing System Simulations

GEOS Global 7 km Nature Run (G5NR)

1. Nature Runs
2. Ocean Radiance Simulation
3. Instrument Simulators



- ◆ G5NR is a non-hydrostatic free-running simulation
- ◆ 30 min timestep
- ◆ 1.5 years
- ◆ Includes GOCART aerosols, O₃, CO, and CO₂

NASA/TM-2014-104606/Vol. 36



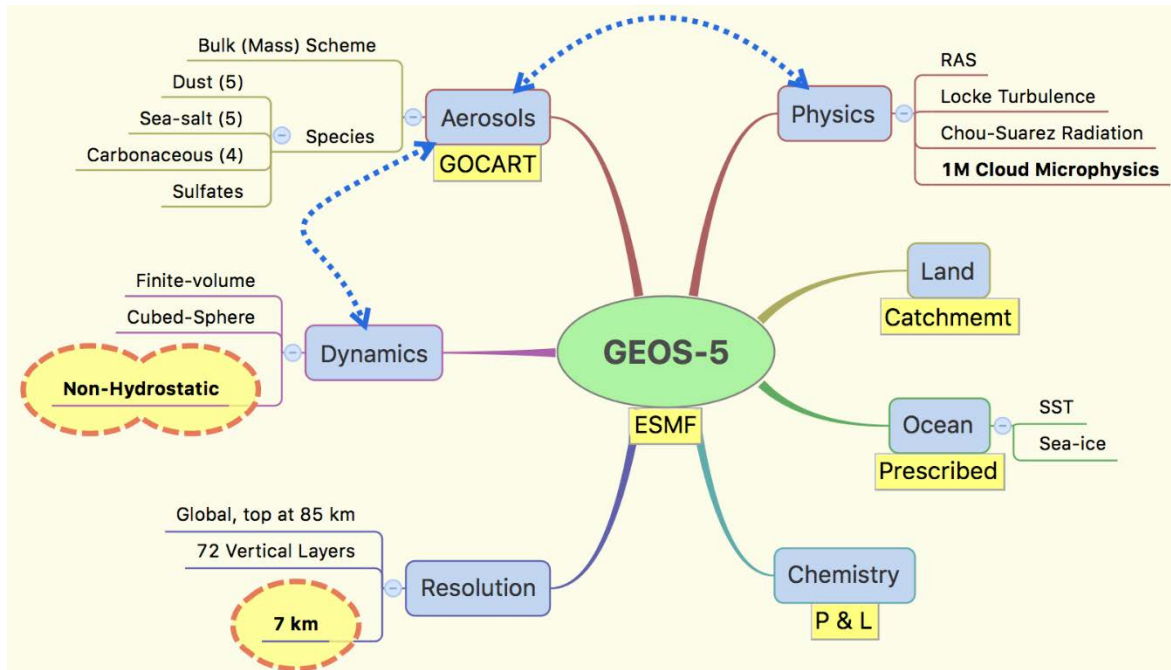
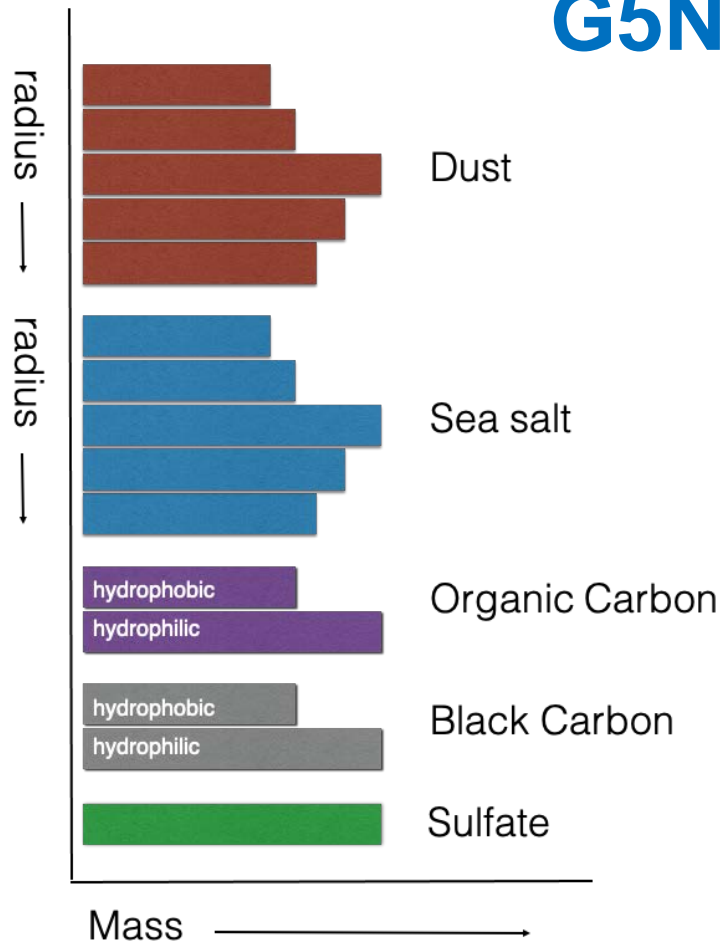
Technical Report Series on Global Modeling and Data Assimilation,
Volume 36

Ronald D. Kniser, Editor

Evaluation of the 7-km GEOS-5 Nature Run

Ronald Colarco, William M. Putnam, Steven Poonen, Clara Deser, Andrea Mikolajewicz, Peter M. Norris, Lindsay Ott, Nelli Prinn, Owen S. Scaife, Deepthi Subbaraj, Michael Branstetter, Virginia Buckland, Winston Chou, Lawrence Coy, Richard Collins, Arindam Das, Anura Datta, Ronald M. Errico, Manojkumar P. Kumar, Min-Jong Kim, Ronald Kniser, Will McCarty, Jyothi Naidu, Gary Poryles, Siegfried Schabert, Guillaume Vernekar, Yuri Yablunovskiy, and Krzysztof Wozniak

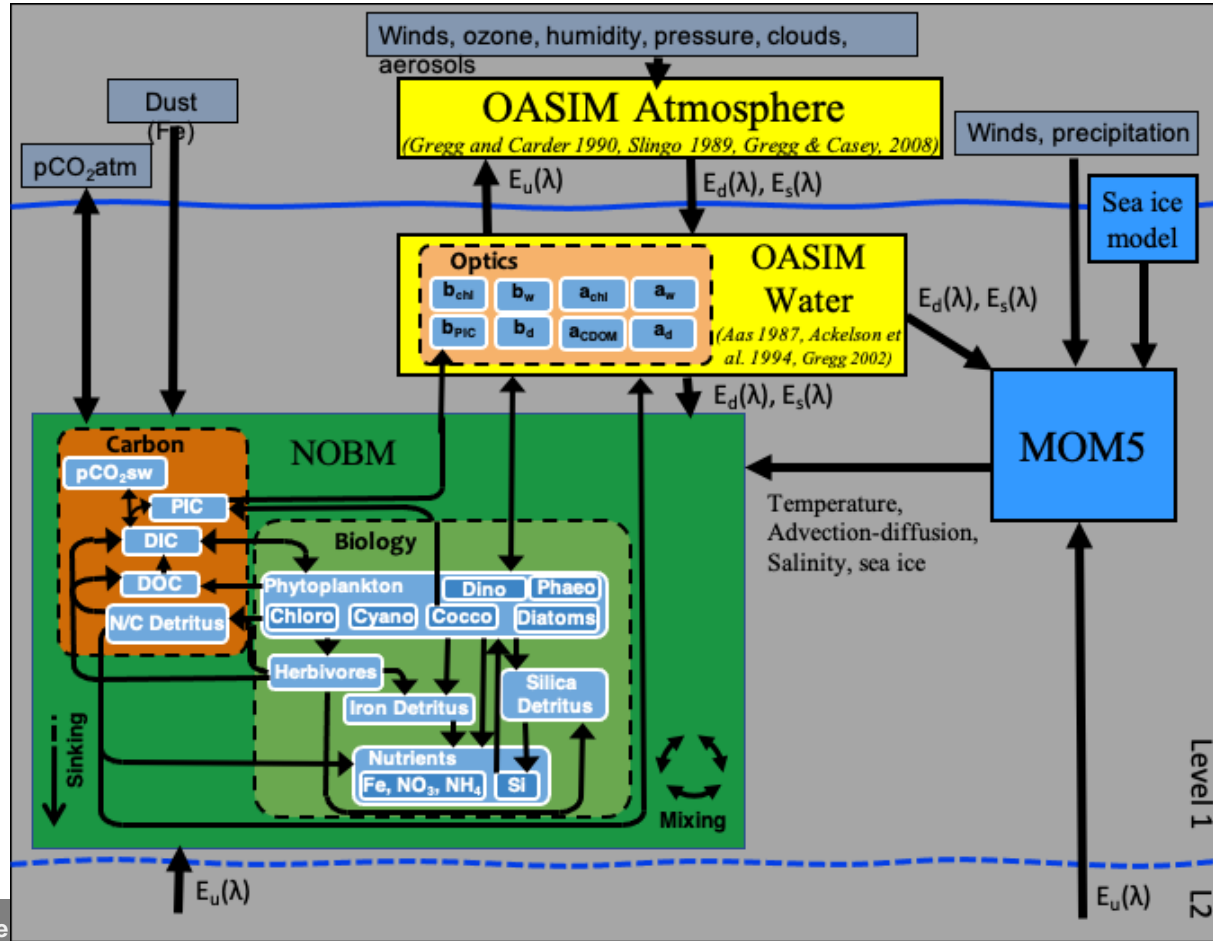
G5NR Configuration



Global Ocean Radiance Simulation

- 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

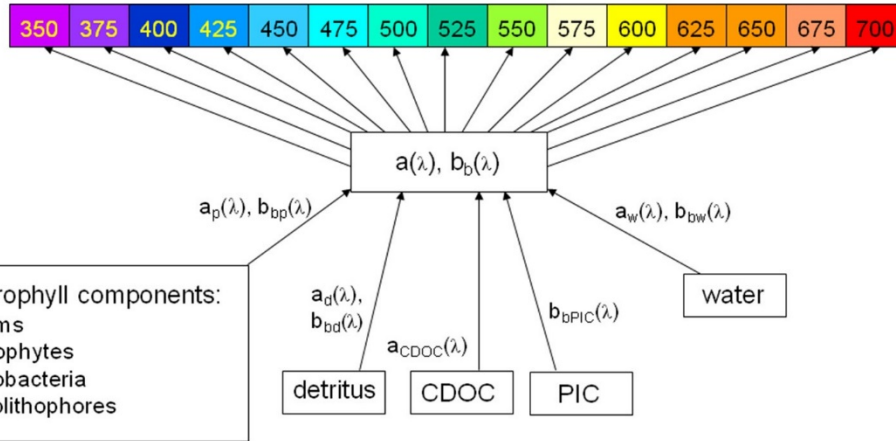
Gregg & Rousseaux, *Frontiers in Marine Science* (2017)



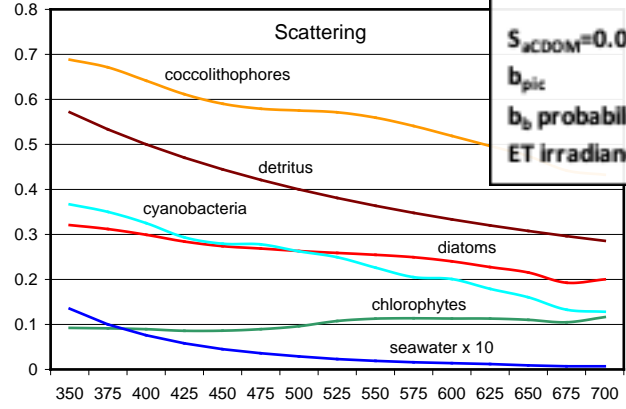
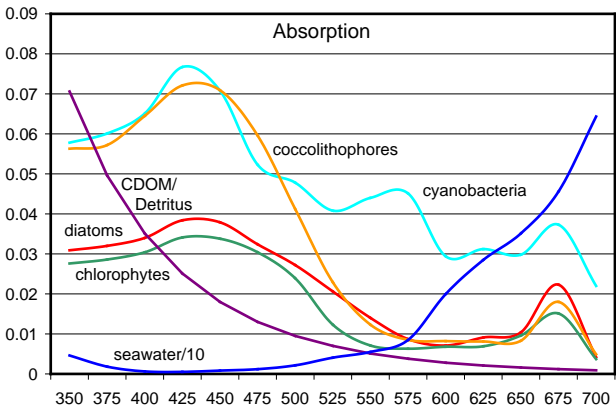


Global Ocean Radiance Simulation

OASIM Upwelling Radiance



a_w, b_w	Smith and Baker 1981 (200-300 nm), (730-800 nm), Morel et al 2007 (325-475), Pope and Fry 1997 (500-720), Circo and Petty 1951 (800nm-2.5um), and Maul 1985 (2.5-4um). Lee et al 2015 (350-550) a_w only
b_b probability	0.5
a_c^+, b_c^+	Morel 1987, Bricaud and Morel 1986 and Bricaud et al. 1988, Ahn et al. 1992 (mass-specific coefficients)
b_b probability (2010)	Ahn et al. 1992, Morel, 1988, Whitmire et al.
a_d^+, b_d^+	Gallegos et al 2011 (mass-specific coefficients)
$S_d=0.013$	Gallegos et al 2011
b_b probability	Gallegos et al 2011
a_{cdom}^+	Yacobi et al 2003; Tzortziou et al 2007 (mass-specific coefficient)
$S_{acDOM}=0.014$	
b_{pic}	Gordon et al 2009
b_b probability	Balch et al 1996
ET irradiance	Thiullier et al 2003





Global Ocean Radiance Simulation

Simulated and Observed Chlorophyll

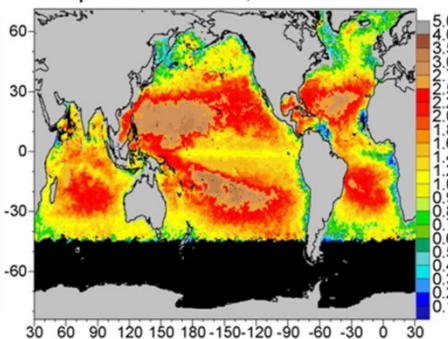
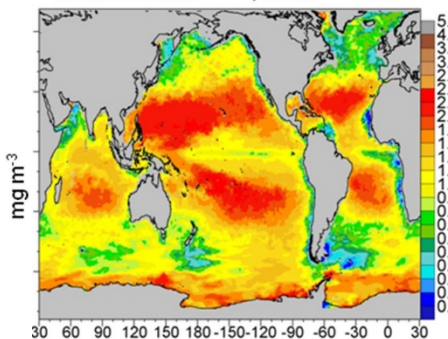
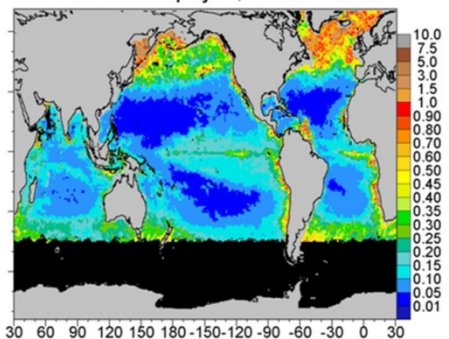
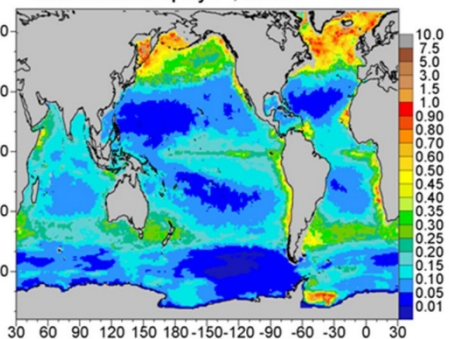
Simulated and Observed Water Leaving Radiance

Model Chlorophyll ; June 2007

MODIS Chlorophyll ; June 2007

Model 412nm ; June 2007

Aqua 412nm ; June 2007

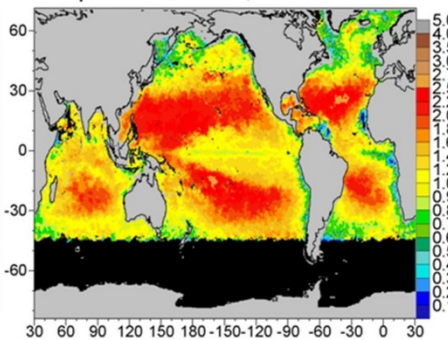
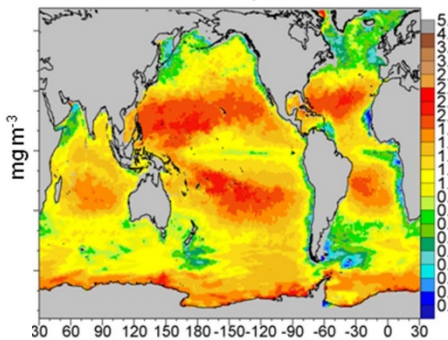
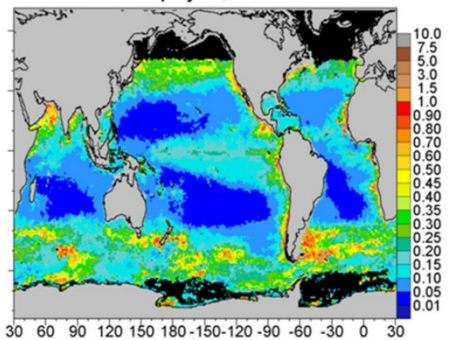
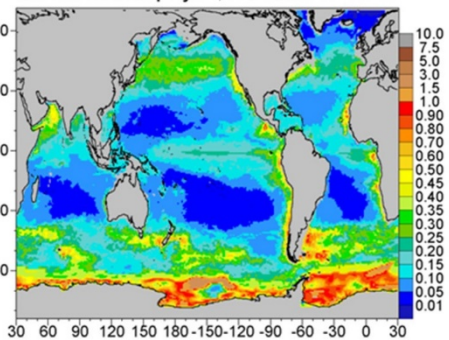


Model Chlorophyll ; December 2007

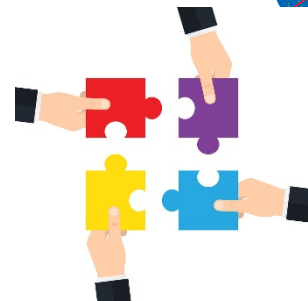
MODIS Chlorophyll ; December 2007

Model 443nm ; June 2007

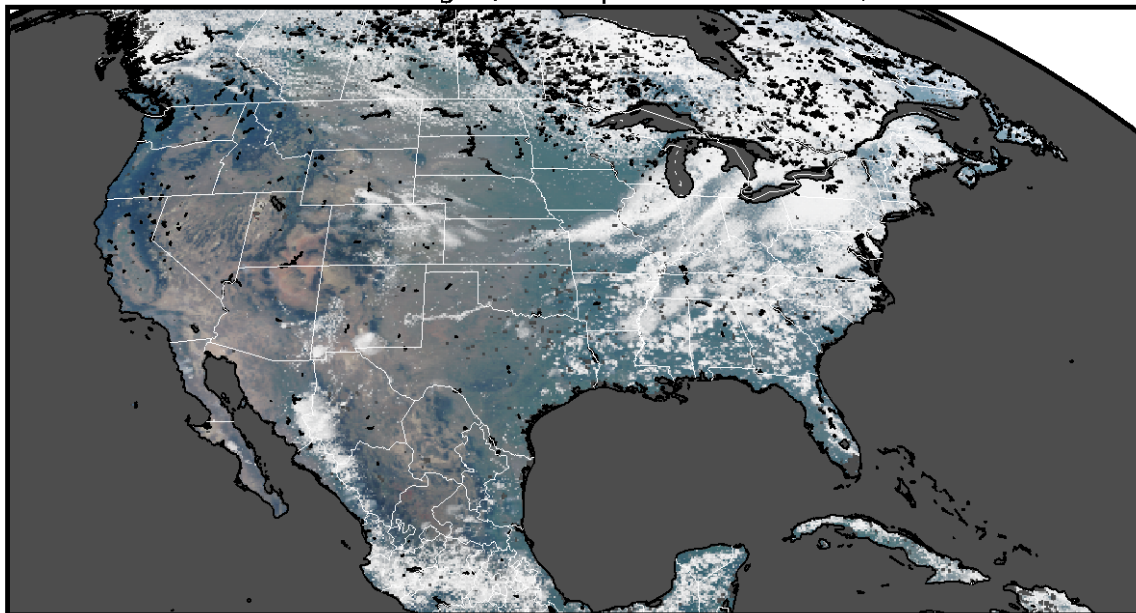
Aqua 443nm ; June 2007



GMAO Instrument Simulator



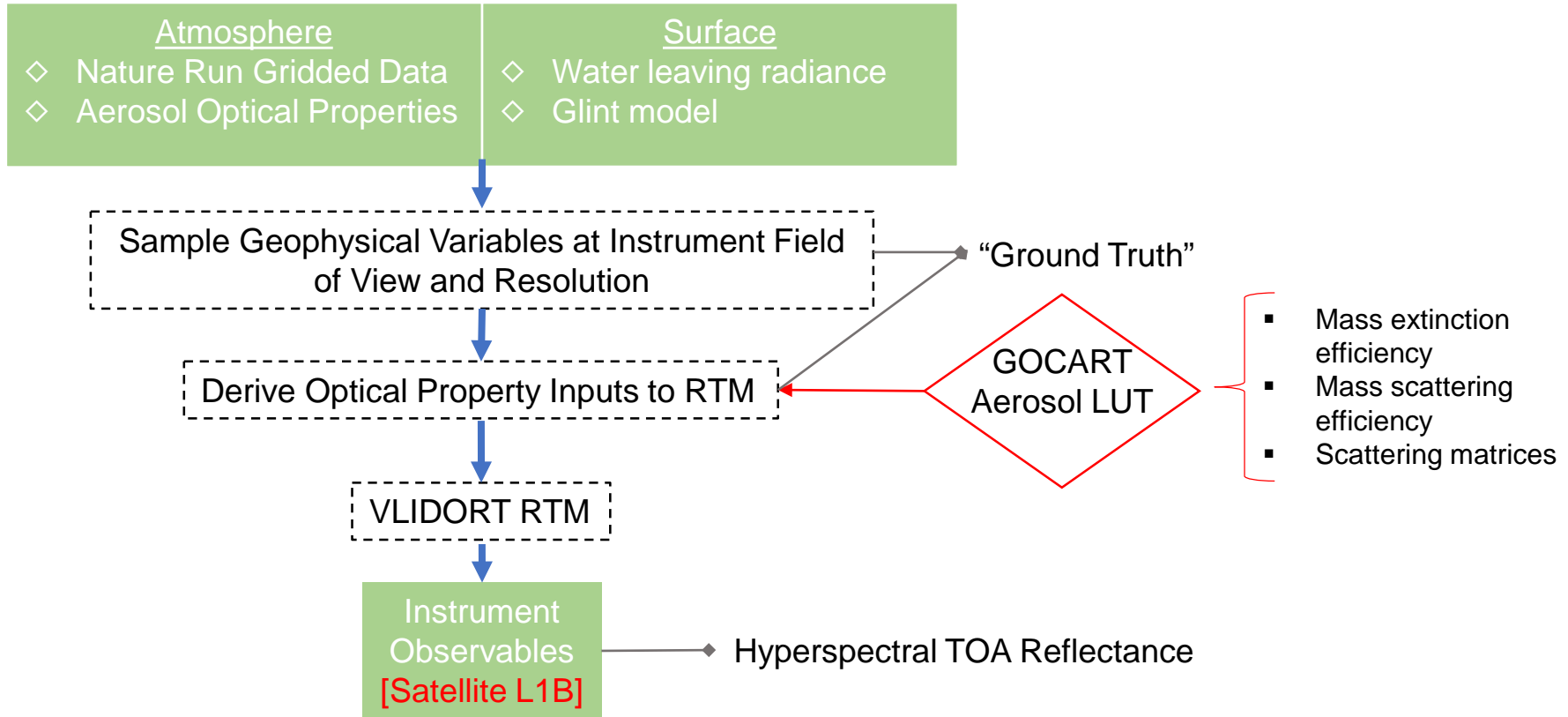
Simulated TEMPO RGB Image



Castellanos, et al. (2019)

- Detailed radiative transfer calculations in the presence of aerosols, clouds, and trace gases
- Apply instrument characteristics (i.e. spectral response)
- Create Simulated Observables:
 - top of the atmosphere radiances
 - backscatter
 - etc.

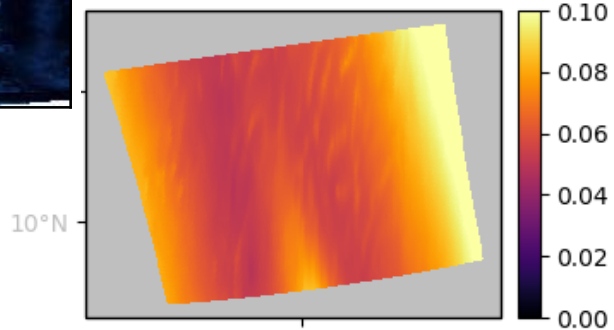
Level 1b Instrument Simulations



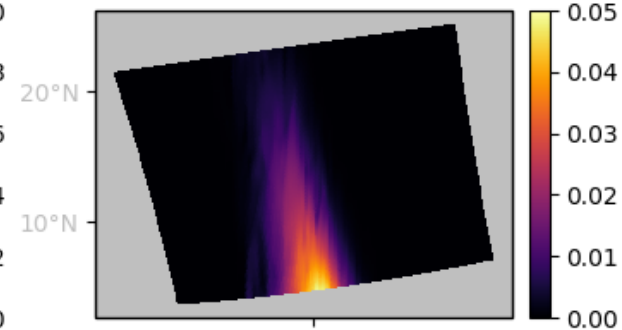
Simulated PACE L1B Granule (V1)



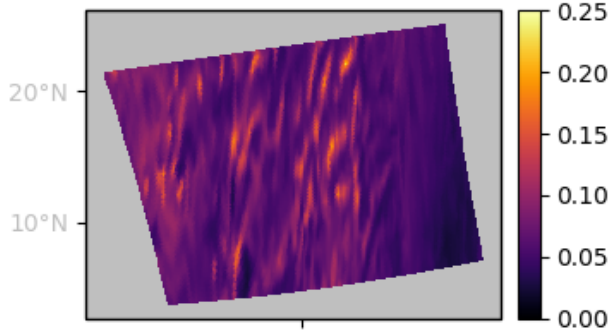
TOA Reflectance 550



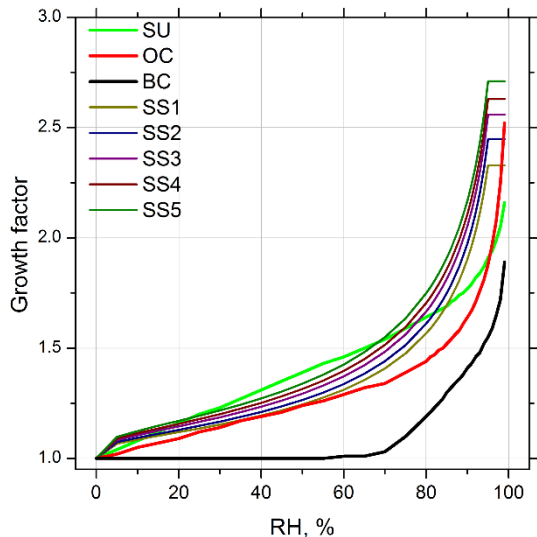
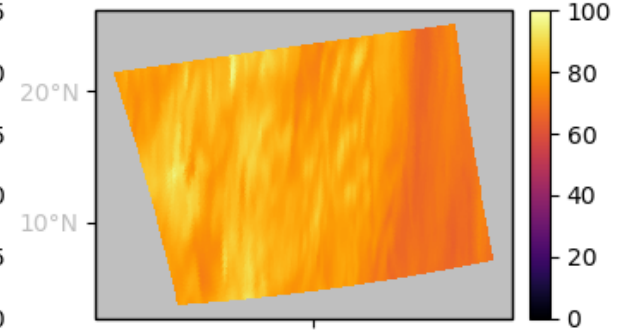
Surface Reflectance 550



G5NR AOD 550



G5NR RH





Simulated PACE L1B Granule

- Data hosted on public website:
 - https://portal.nccs.nasa.gov/datashare/G5NR/c1440_NR/OBS/PACE
- Organized by Levels
 - LevelA: Raw inputs (very large datasets)
 - LevelB: Inputs subsampled to PACE granule
 - e.g. T, P, RH, aerosol mass profiles
 - LevelC: RTM optical input/outputs
 - e.g. Rayleigh optical depth, AOD, surface reflectance, TOA radiance
 - LevelC2: TOA radiance in PACE L1B file format
- Version 1
 - 5 nm step
 - No trace gas absorption



Required OCI Science Products

Required Products with Uncertainty Requirements

Water Leaving Reflectance (350, 360, 385, 412, 425, 443, 460, 475, 490, 510, 532, 555, 583, 617, 640, 655, 665, 678, 710 nm)

AOD at 380, 440, 500, 550, and 675 nm

Fraction of AOD(550) from fine mode aerosols over oceans

Cloud layer detection for optical depth > 0.3

Cloud top pressure of opaque (optical depth > 3) clouds

Water path of liquid, ice clouds

Optical thickness of liquid clouds

Effective radius of liquid clouds

Optical thickness of ice clouds

Effective radius of ice clouds

Shortwave radiative effect

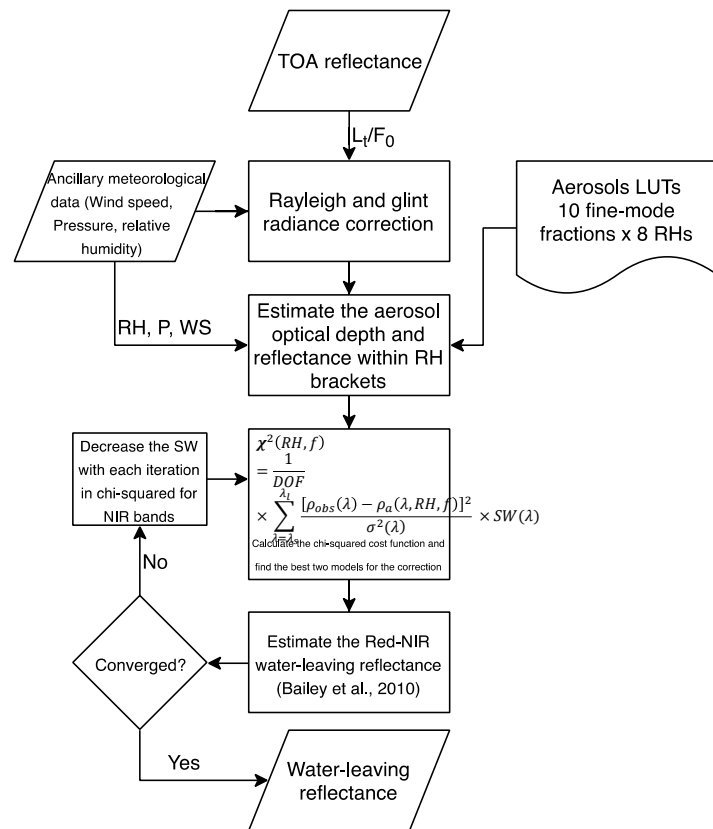
- OCI required products define mission success and drive OCI design
- PACE Project has plan for production of all required data products
 - Based on MODIS & VIIRS heritage algorithms
 - Ocean Color
 - Aerosols

OCI Aerosol and Ocean Color Algorithms

■ Aerosol: Dark Target/Deep Blue

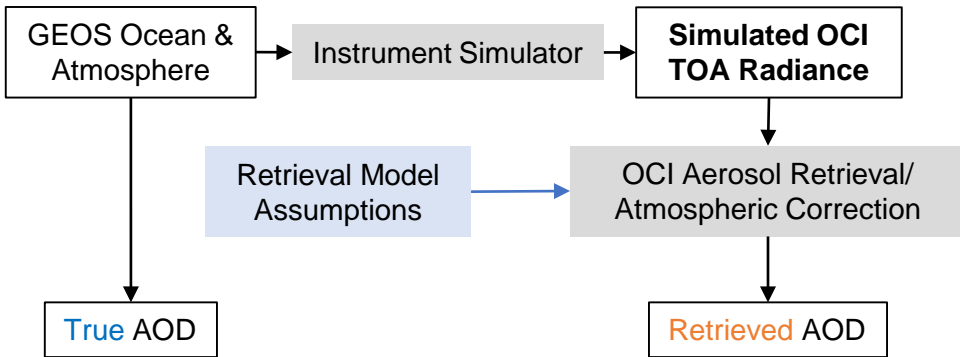
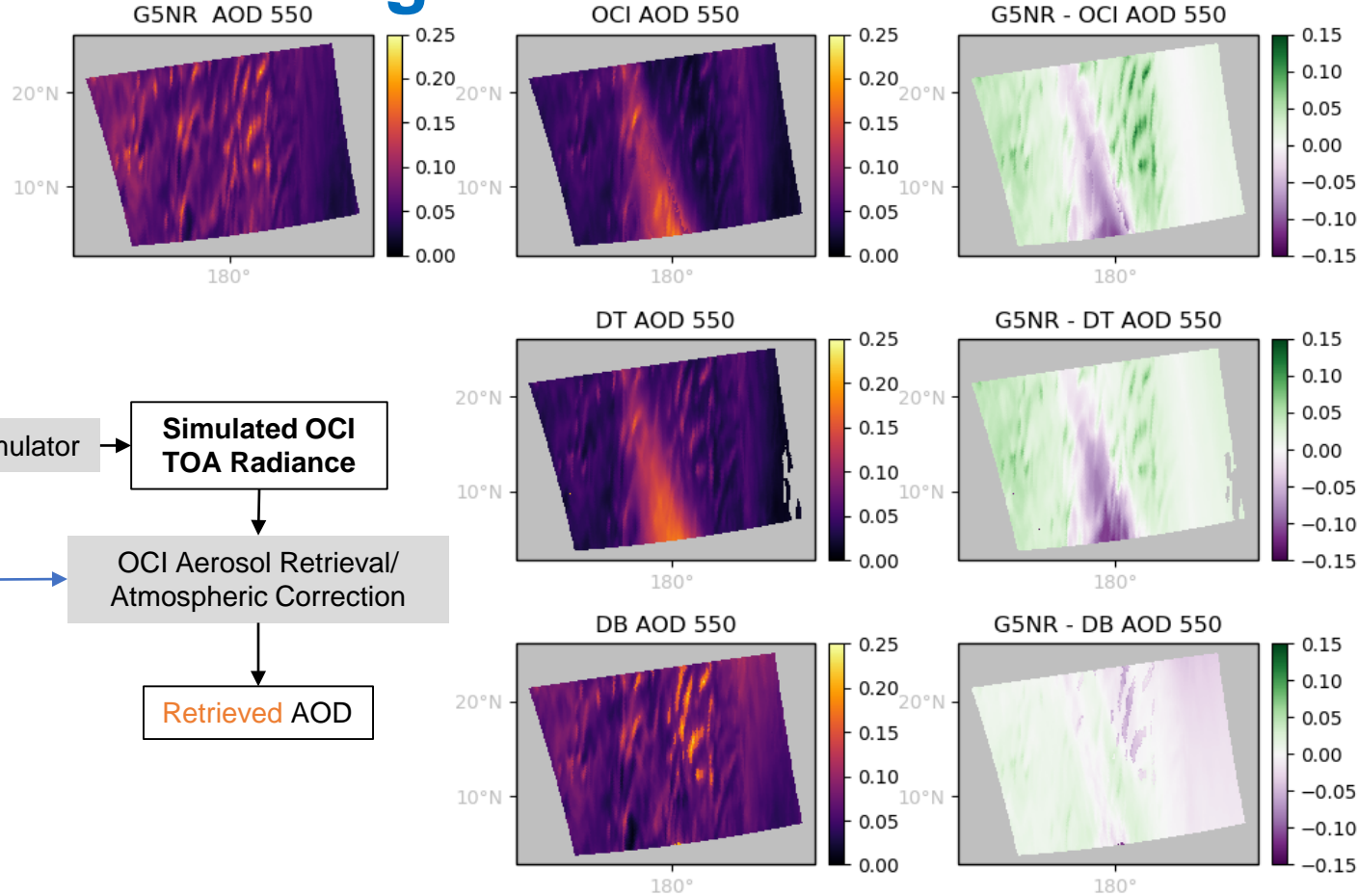
- PACE SDS have a modular framework for implementing aerosol algorithms
 - Able to swap cloud mask components, etc
- MODIS/VIIRS aerosol algorithms implemented in PACE proxy chain
 - Run at full L1 resolution as opposed to the coarser L2 MODIS/VIIRS default

■ Ocean Color

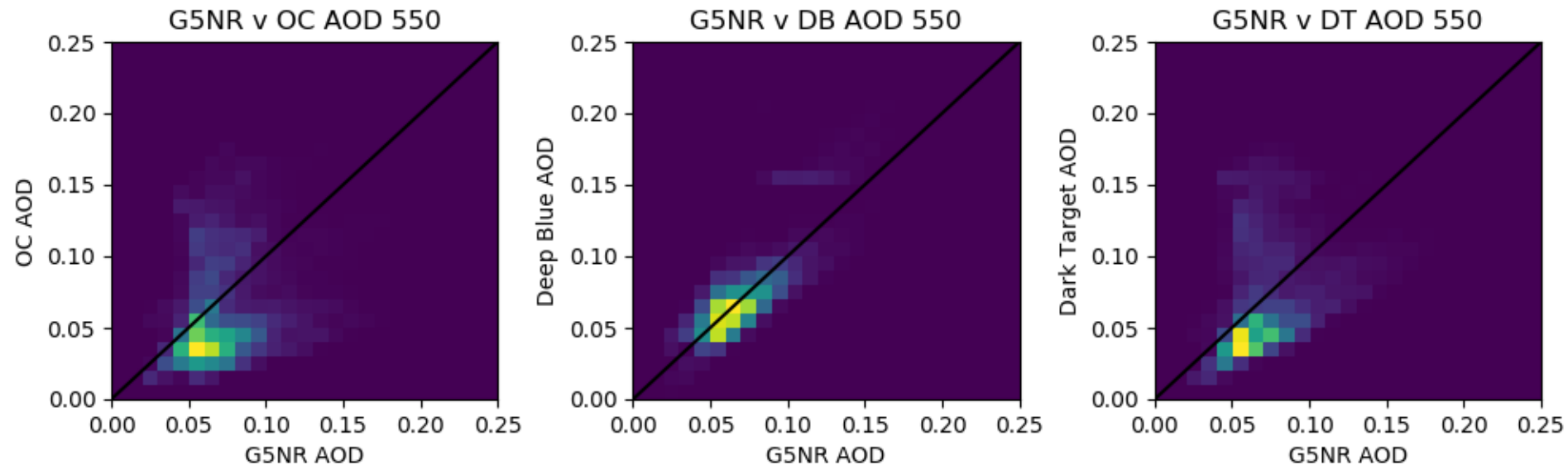




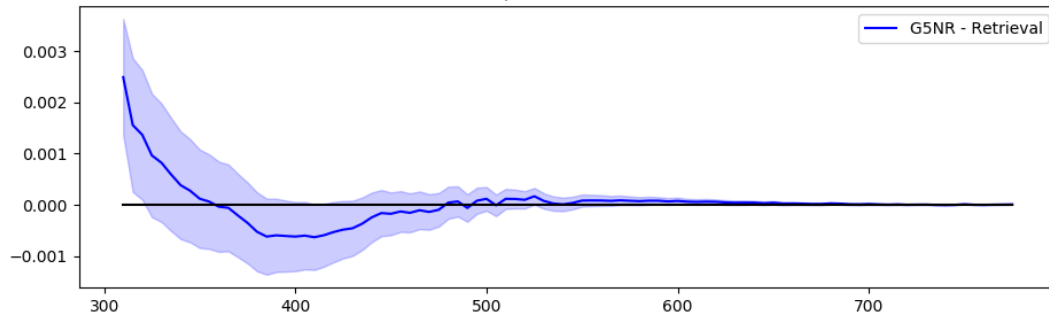
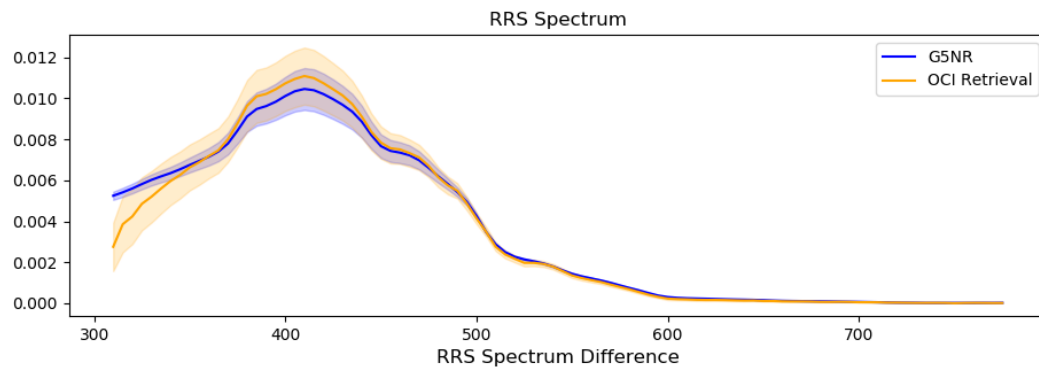
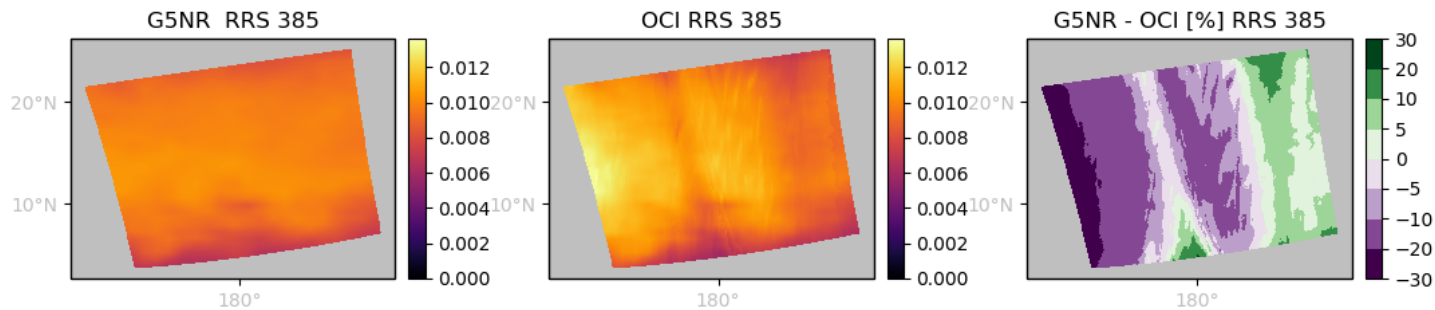
Simulated Data Applied to OCI Aerosol & Ocean Color Algorithms



AOD Comparisons

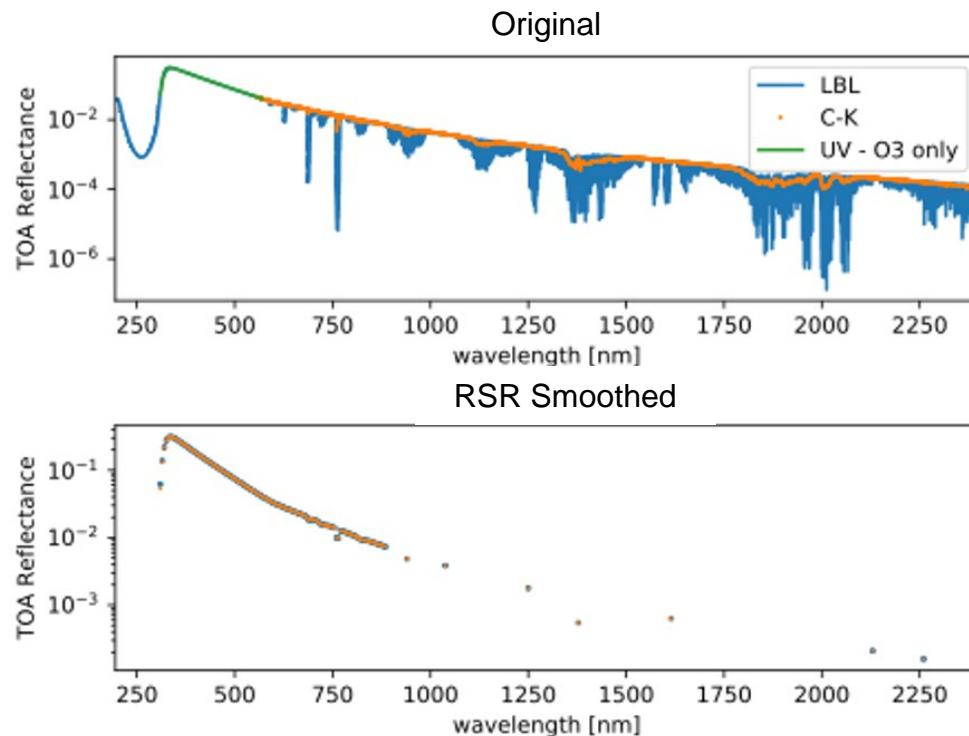


Ocean Color Retrieval



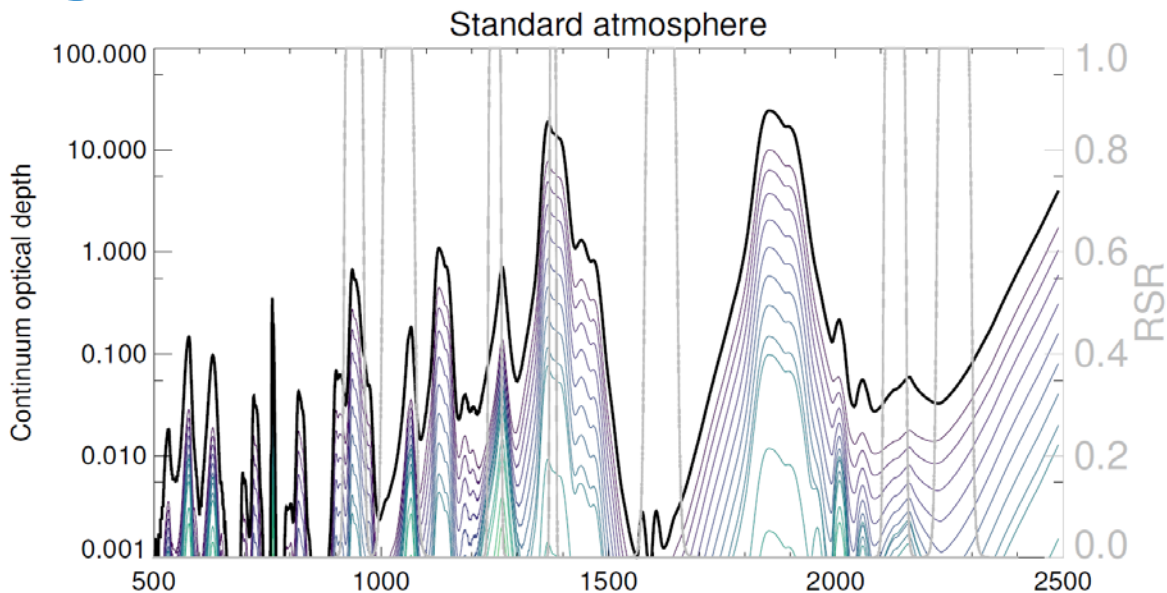
Version 2: Hyperspectral Trace Gas Absorption

- Using ~1,000 spectral channels
 - < 0.25% error compared to LBL (Line by line absorption comes from HITRAN 2012)
- Includes major absorbing gases: CO, CO₂, O₃, H₂O, CH₄, N₂O, O₂
 - CO, CO₂, O₃ and H₂O from G5NR (dynamic)
 - Rest climatological means
- Have analyzed AC on a small fraction of the OCI granule
 - Will start full granule simulation imminently (takes ~4 days)



Version 3: trace gas absorption continuum

- Working on adding MT_CKD v3.3 (H_2O , O_2 , CO_2 , N_2)
- Increases absorption optical depth most in strongly absorbing bands (H_2O , O_2)
- Non-negligible presence in 2.x microns as well (optical depth ~ 0.03)



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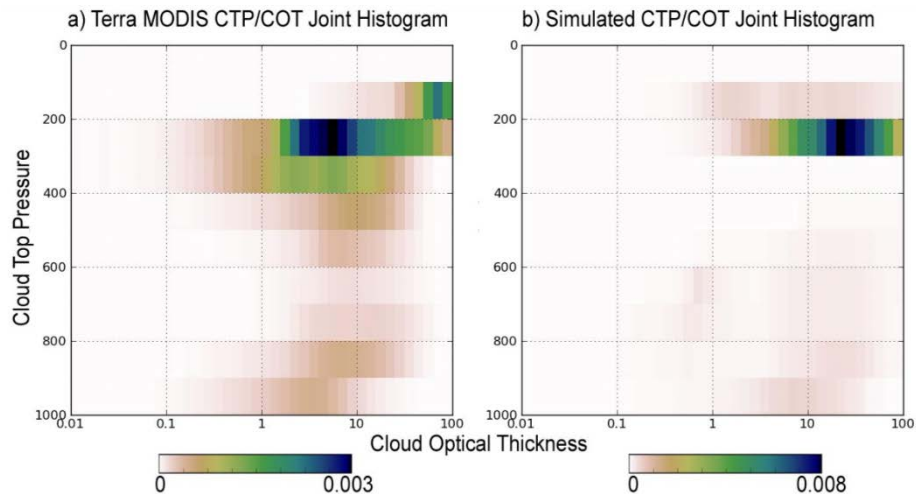
Phil. Trans. R. Soc. A (2012) **370**, 2520–2556
doi:10.1098/rsta.2011.0295

Development and recent evaluation of the MT_CKD model of continuum absorption

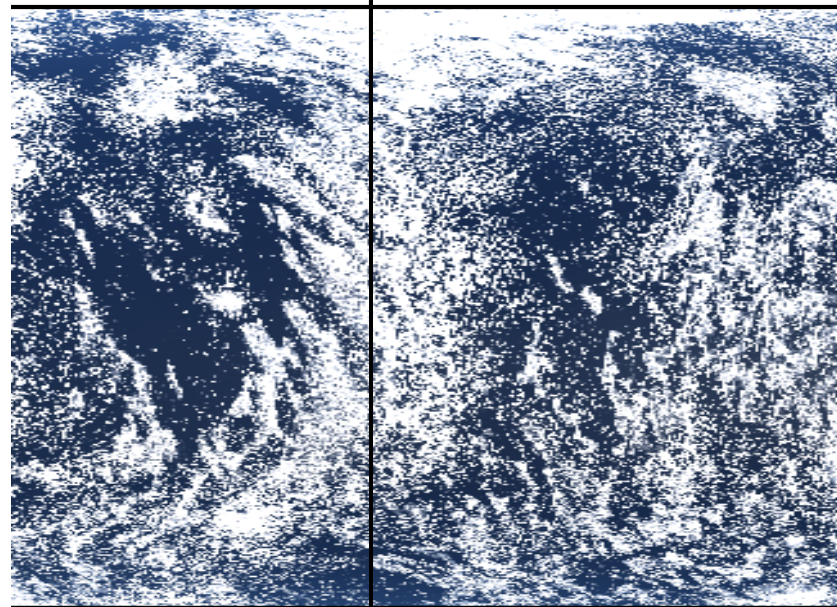
BY ELI J. MLAWER^{1,*}, VIVIENNE H. PAYNE^{1,†}, JEAN-LUC MONCET¹,
JENNIFER S. DELAMERE^{1,‡}, MATTHEW J. ALVARADO¹ AND DAVID C. TOBIN²

Version 4: Clouds

- GMAO has developed a downscaling algorithm to create realistic cloud optical depth distributions from bulk moisture fields
- Has been used in MODIS cloud retrieval studies (Wind et al. 2013)



Cloudy RGB Simulation



Norris et al. "Representation of 3D heterogeneous cloud fields using copulas: Theory for water clouds", QJRMS, 2008.



Summary

- GMAO's high fidelity Earth system modeling of atmosphere and ocean constituents are a useful tool for PACE algorithm development and testing
- GMAO is developing instrument simulators that are the forward operators between geophysical variables and satellite observables
- This work requires detailed validation/benchmarking along the way to ensure viable error tolerances

- This is a work in progress, more retrieval algorithm analysis to come.
- Will produce 1 orbit of Versions 2-4
 - Interested in feedback from the SAT on additional locations/times of year that would be of interest.