PACE R_{rs} Uncertainty

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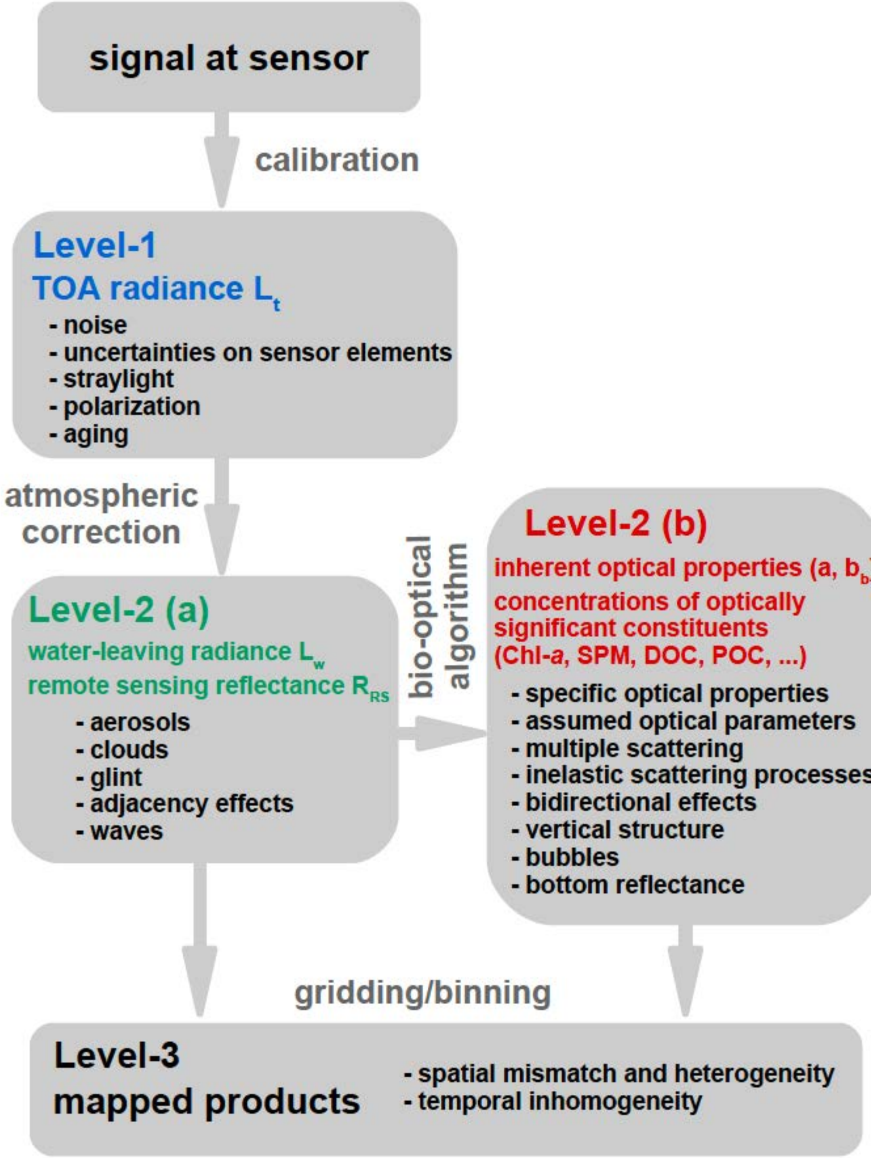
Sources of uncertainties in ocean color

- Radiometric uncertainty
  - Random noise → SNR.
  - Systematic uncertainty (calibration errors).
- Non-radiometric
  - Geolocation accuracy
  - Band-to-band registration
- Modeling uncertainty
  - Radiative transfer errors.
  - Simplification of physics.

Pre-launch and on-orbit calibration



signal at sensor

calibration

Level-1
TOA radiance L_t
- noise
- uncertainties on sensor elements
- straylight
- polarization
- aging

atmospheric correction

Level-2 (a)
water-leaving radiance L_w
remote sensing reflectance R_{RS}
- aerosols
- clouds
- glint
- adjacency effects
- waves

bio-optical algorithm

Level-2 (b)
inherent optical properties (a, b_b
concentrations of optically significant constituents (Chl-*a*, SPM, DOC, POC, ...)
- specific optical properties
- assumed optical parameters
- multiple scattering
- inelastic scattering processes
- bidirectional effects
- vertical structure
- bubbles
- bottom reflectance

gridding/binning

Level-3
mapped products
- spatial mismatch and heterogeneity
- temporal inhomogeneity

IOCCG, report 18

20+ years of diagnostic uncertainty estimates in ocean color

- Pixel-level uncertainty has been absent from the ocean color community for decades.
- The community relies on the validation data to provide diagnostic estimates of uncertainty.
- Validation data is not representative of the global oceans.
- Uncertainty varies spatially and temporal (season).

Product Name	MODIS Aqua Range	In situ Range	#	Best Fit Slope	Best Fit Intercept	R^2	Median Ratio	Abs % Difference	RMSE
Rrs412	-0.00411, 0.01820	0.00000, 0.01964	1945	1.03539	-0.00065	0.90481	0.90307	22.21457	0.00147
Rrs443	-0.00065, 0.01950	0.00005, 0.01783	1774	1.04628	-0.00026	0.88967	1.00894	12.06771	0.00109
Rrs488	0.00033, 0.02513	0.00039, 0.02289	2127	0.94853	-0.00021	0.89894	0.91509	12.00520	0.00106
Rrs531	0.00092, 0.01682	0.00130, 0.02110	639	0.87525	0.00017	0.91346	0.97562	11.98040	0.00096
Rrs547	0.00088, 0.01590	0.00091, 0.01984	469	0.91611	0.00018	0.92442	1.04480	13.38668	0.00072
Rrs667	-0.00016, 0.01186	0.00002, 0.01100	709	0.98687	-0.00002	0.91982	0.94565	37.48856	0.00017
Rrs678	-0.00015, 0.00283	0.00004, 0.00295	373	0.94854	-0.00000	0.89380	1.00161	32.16394	0.00008

The linear regression algorithm has been changed to reduced major axis.

PACE SDT Goal for Rrs(VIS)

ΔR_{rs}(VIS) = 3e-4 sr^{-1} or 5%

Current Approach

ΔR_{rs}(VIS) ~ 1e-3 sr^{-1} or 12% (22% 412)

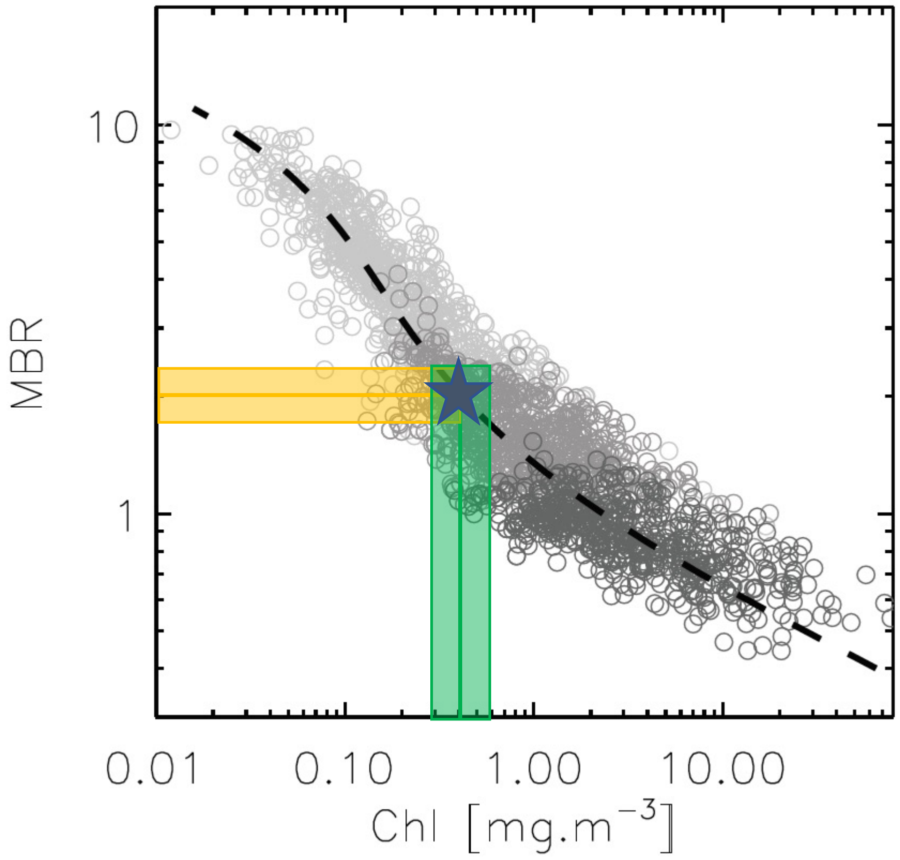
goal is factor of 3 reduction ... seems achievable!

Toward pixel-level uncertainty in operational products

- There are various methods to estimate the pixel-level uncertainty:
  - Monte Carlo sampling
  - Analytical error propagation
  - Bayesian Framework (Optimal Estimation)
  - Machine learning (ensemble approach)
  - Cramér-Rao Bounds
  - …

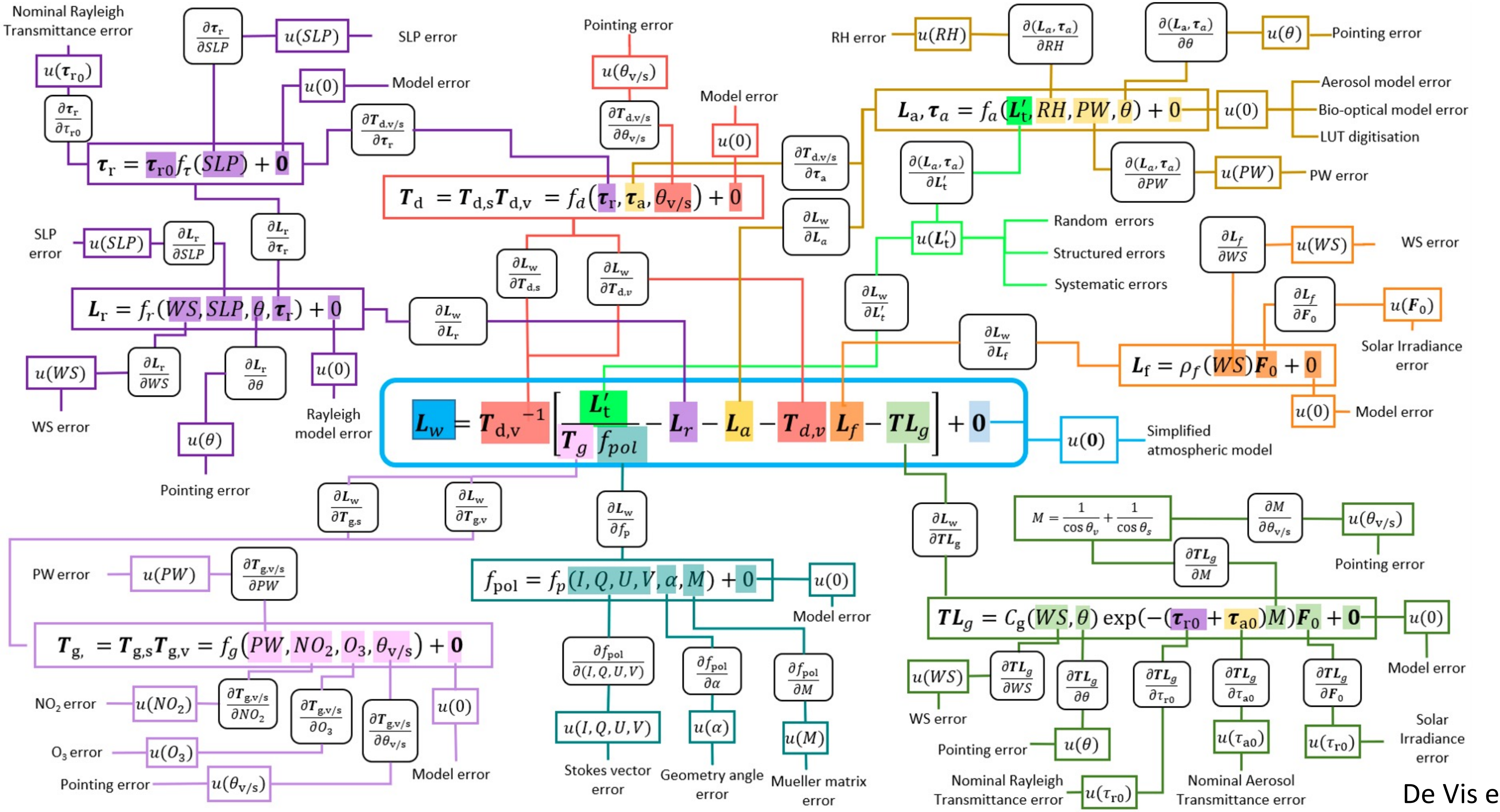
$$y = f(x_1, x_1, \ldots, x_n)$$

$$u^2\,(y) = \sum_{i=\text{`}}^{n} \left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i) + 2\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} \frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j} u(x_i, x_i)$$



Pixel-level uncertainty in SeaDAS

$$L_t(\lambda) = \Big(L_r(\lambda) + L_a(\lambda) + L_{ra}(\lambda) + t(\lambda)L_f(\lambda) + T(\lambda)L_g(\lambda) + t(\lambda)L_w(\lambda)\Big)\times T_g(\lambda)$$



Nominal Rayleigh Transmittance error

$u(\tau_{r0})$

$\frac{\partial \tau_r}{\partial \tau_{r0}}$

$\frac{\partial \tau_r}{\partial SLP}$

$u(SLP)$

SLP error

$u(0)$

Model error

$\tau_r = \tau_{r0} f_\tau(SLP) + 0$

$\frac{\partial T_{d,v/s}}{\partial \tau_r}$

Pointing error

$u(\theta_{v/s})$

$\frac{\partial T_{d,v/s}}{\partial \theta_{v/s}}$

Model error

$u(0)$

$T_d = T_{d,s}T_{d,v} = f_d(\tau_r, \tau_a, \theta_{v/s}) + 0$

$\frac{\partial T_{d,v/s}}{\partial \tau_a}$

$\frac{\partial L_w}{\partial L_a}$

RH error

$u(RH)$

$\frac{\partial (L_a, \tau_a)}{\partial RH}$

$\frac{\partial (L_a, \tau_a)}{\partial \theta}$

$u(\theta)$

Pointing error

$L_a, \tau_a = f_a(L'_t, RH, PW, \theta) + 0$

$u(0)$

Aerosol model error

Bio-optical model error

LUT digitisation

$\frac{\partial (L_a, \tau_a)}{\partial L'_t}$

$\frac{\partial (L_a, \tau_a)}{\partial PW}$

$u(PW)$

PW error

$u(L'_t)$

Random errors

Structured errors

Systematic errors

$\frac{\partial L_f}{\partial WS}$

$u(WS)$

WS error

$\frac{\partial L_f}{\partial F_0}$

$u(F_0)$

Solar Irradiance error

$\frac{\partial L_w}{\partial L'_t}$

$\frac{\partial L_w}{\partial L_f}$

$L_f = \rho_f(WS)F_0 + 0$

$u(0)$

Model error

SLP error

$u(SLP)$

$\frac{\partial L_r}{\partial SLP}$

$\frac{\partial L_r}{\partial \tau_r}$

$L_r = f_r(WS, SLP, \theta, \tau_r) + 0$

$\frac{\partial L_w}{\partial L_r}$

$\frac{\partial L_w}{\partial T_{d,s}}$

$\frac{\partial L_w}{\partial T_{d,v}}$

$u(WS)$

WS error

$\frac{\partial L_r}{\partial WS}$

$\frac{\partial L_r}{\partial \theta}$

$u(0)$

Rayleigh model error

$u(\theta)$

Pointing error

$$L_w = T_{d,v}^{-1}\left[\frac{L'_t}{T_g\, f_{pol}} - L_r - L_a - T_{d,v}L_f - TL_g\right] + 0$$

$u(0)$

Simplified atmospheric model

$\frac{\partial L_w}{\partial T_{g,s}}$

$\frac{\partial L_w}{\partial T_{g,v}}$

$\frac{\partial L_w}{\partial f_p}$

$\frac{\partial L_w}{\partial TL_g}$

PW error

$u(PW)$

$\frac{\partial T_{g,v/s}}{\partial PW}$

$T_g = T_{g,s}T_{g,v} = f_g(PW, NO_2, O_3, \theta_{v/s}) + 0$

NO_2 error

$u(NO_2)$

$\frac{\partial T_{g,v/s}}{\partial NO_2}$

$\frac{\partial T_{g,v/s}}{\partial O_3}$

$\frac{\partial T_{g,v/s}}{\partial \theta_{v/s}}$

$u(0)$

Model error

O_3 error

$u(O_3)$

Pointing error

$u(\theta_{v/s})$

$f_{pol} = f_p(I, Q, U, V, \alpha, M) + 0$

$u(0)$

Model error

$\frac{\partial f_{pol}}{\partial (I,Q,U,V)}$

$u(I,Q,U,V)$

Stokes vector error

$\frac{\partial f_{pol}}{\partial \alpha}$

$u(\alpha)$

Geometry angle error

$\frac{\partial f_{pol}}{\partial M}$

$u(M)$

Mueller matrix error

$M = \frac{1}{\cos\theta_v} + \frac{1}{\cos\theta_s}$

$\frac{\partial M}{\partial \theta_{v/s}}$

$u(\theta_{v/s})$

Pointing error

$\frac{\partial TL_g}{\partial M}$

$TL_g = C_g(WS, \theta)\exp(-(\tau_{r0} + \tau_{a0})M)F_0 + 0$

$u(0)$

Model error

$u(WS)$

WS error

$\frac{\partial TL_g}{\partial WS}$

$\frac{\partial TL_g}{\partial \theta}$

Pointing error

$u(\theta)$

$\frac{\partial TL_g}{\partial \tau_{r0}}$

Nominal Rayleigh Transmittance error

$u(\tau_{r0})$

$\frac{\partial TL_g}{\partial \tau_{a0}}$

$u(\tau_{a0})$

Nominal Aerosol Transmittance error

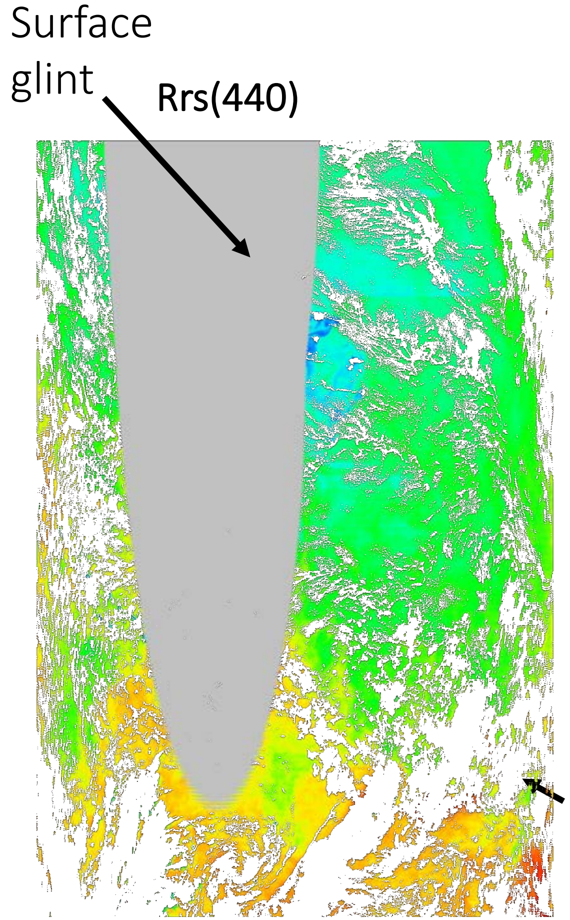
$\frac{\partial TL_g}{\partial F_0}$

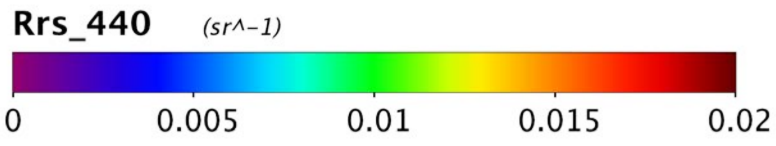
$u(\tau_{r0})$

Solar Irradiance error

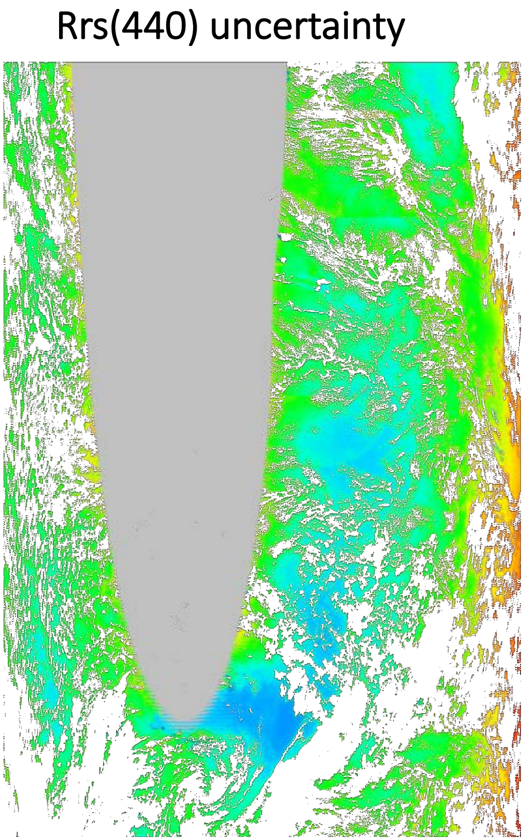
De Vis et al (2022)

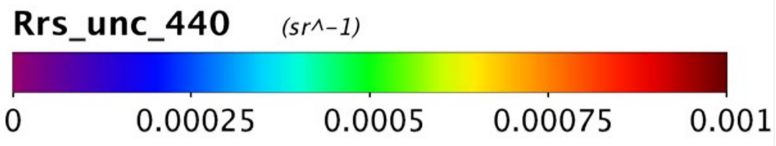
Pixel-level uncertainty of OCI



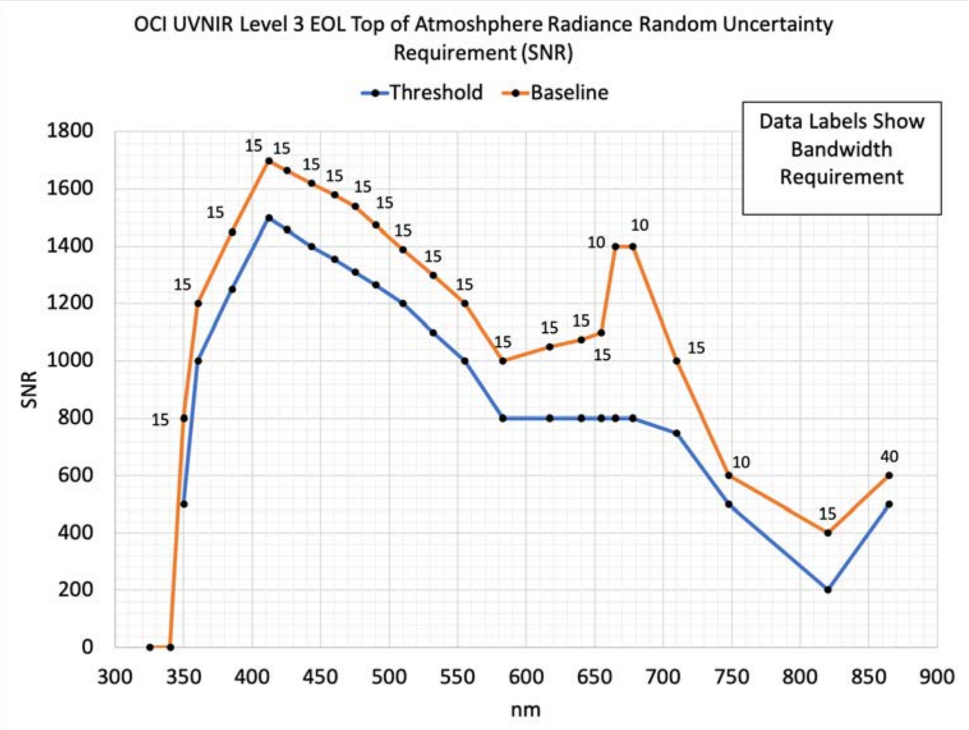


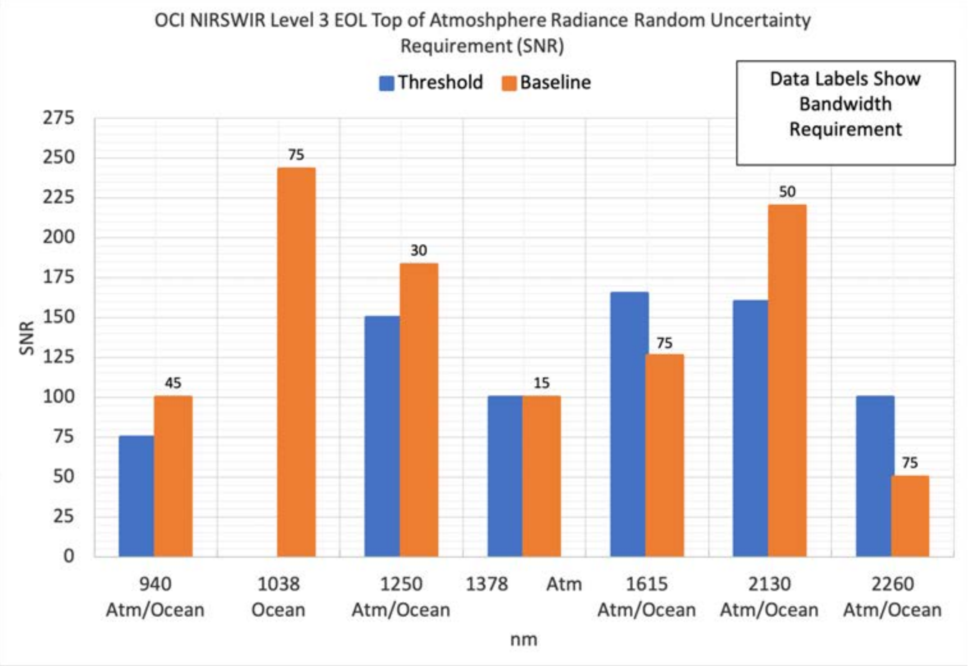
One goal is to retrieve Rrs_unc_440 < 0.00076 sr-1





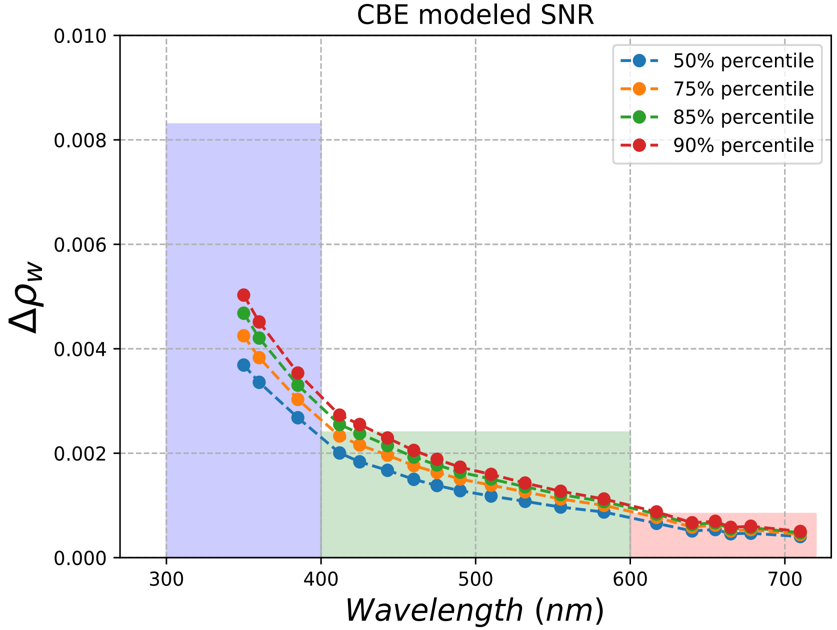
Rrs_unc here includes random noise + systematic unc. + forward model unc.





Pre-launch instrument uncertainty model tells us how well we will do for PACE

Data Product	Baseline Uncertainty
Water-leaving reflectances centered on (±2.5 nm) 350, 360, and 385 nm (15 nm bandwidth)	0.0057 or 20%
Water-leaving reflectances centered on (±2.5 nm) 412, 425, 443, 460, 475, 490, 510, 532, 555, and 583 (15 nm bandwidth)	0.0020 or 5%
Water-leaving reflectances centered on (±2.5 nm) 617, 640, 655, 665 678, and 710 (15 nm bandwidth, except for 10 nm bandwidth for 665 and 678 nm)	0.0007 or 10%

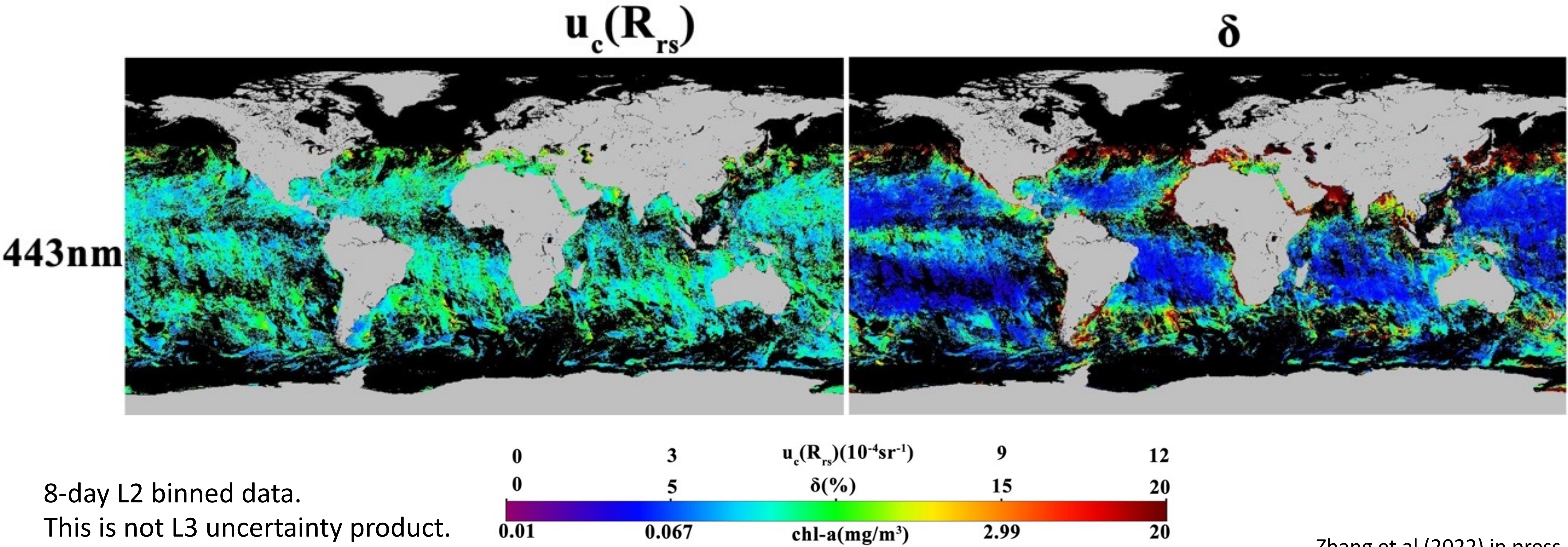


Uncertainty in ocean reflectance after the Atmospheric Correction

- ✓ Remember there are requirements that we need to meet for the water reflectance.
- ✓ Remember that we can use our global PyTOAST simulations to test these requirments

Are we going to produce operational uncertainty products? yes

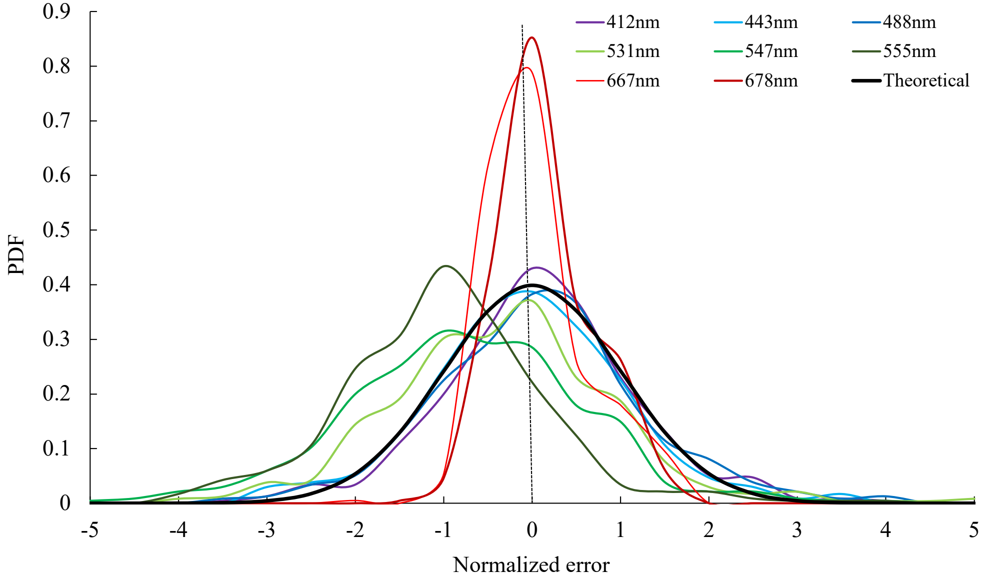
- We will be able to produce Rrs and IOPs uncertainty for L2 products from PACE and other heritage sensors.

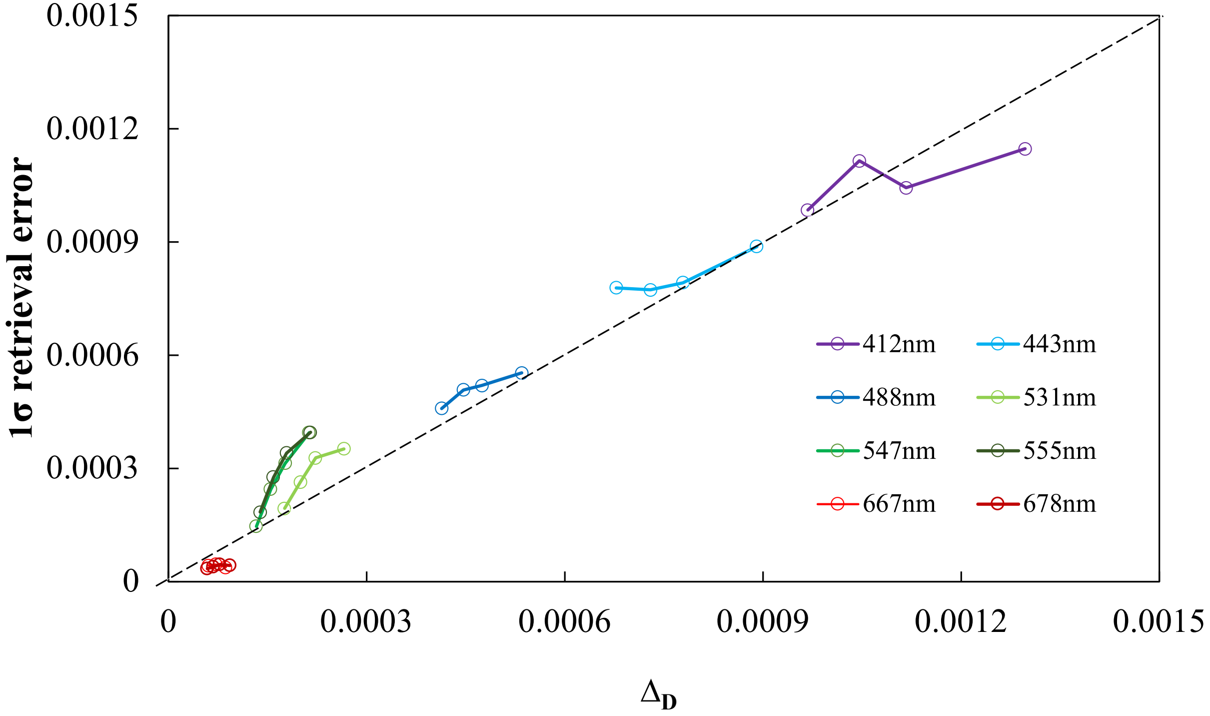


8-day L2 binned data.
This is not L3 uncertainty product.

Zhang et al (2022) in press

Validating the pixel-level uncertainty





$$\Delta_N = \frac{R_{rs}^{m} - R_{rs}^{f}}{\Delta_D}$$

Zhang et al (2022) in press

Probabilistic/Bayesian Optimal Estimation Framework

- Developed a Bayesian version of the full-spectrum AC (combined with the GIOP forward ocean model).
  - Define the state vector:

$$\mathbf{x} = [\underbrace{\overbrace{RH, O_3, Pr, WS, WV}^{\text{Ancillary with strongly informative priors}}, fmf, \tau_a}_{\textbf{Atmosphere}\text{ parameters}}, \underbrace{a_{ph}, a_{dg}, b_{bp}}_{\text{GIOP }\textbf{ocean}\text{ parameters}}]$$

  - Define the objective function:

$$\chi^2 = [\boldsymbol{\rho}_{obs} - \mathbf{F}(\boldsymbol{x})]^T \mathbf{S}_e^{-1} [\boldsymbol{\rho}_{obs} - \mathbf{F}(\boldsymbol{x})] + [\boldsymbol{x} - \boldsymbol{x}_a]^T \mathbf{S}_a^{-1} [\boldsymbol{x} - \boldsymbol{x}_a]$$

  - Optimize the objective function given the forward model to estimate the state vector.

$$\rho_{TOA}(\lambda, \theta_0, \varphi, \theta_v) = \mathbf{F}(RH, O_3, Pr, WS, WV, fmf, \tau_a, a_{ph}, a_{dg}, b_{bp}, \gamma, Chl - a)$$

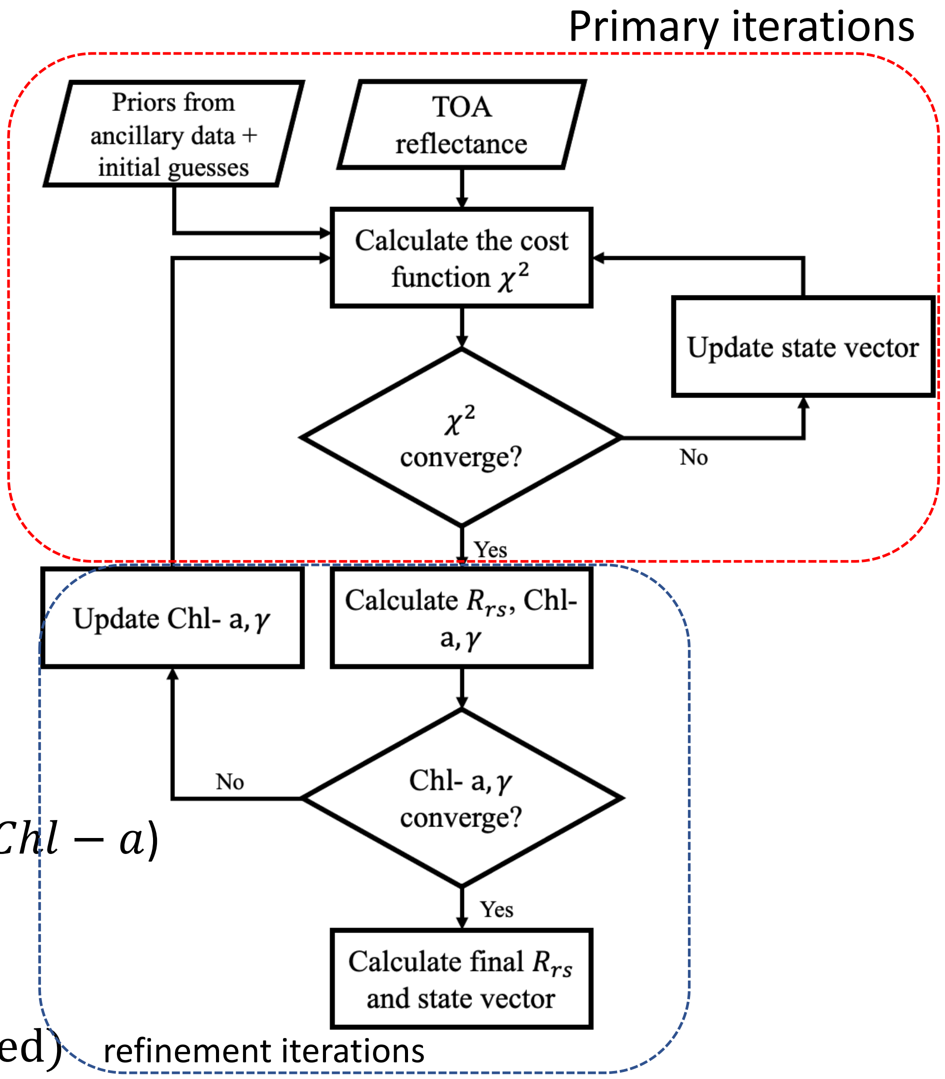
  - Estimate the error covariance matrix:

$$\hat{\mathbf{S}} = \left(\hat{\mathbf{K}}^T \mathbf{S}_e^{-1} \hat{\mathbf{K}} + \mathbf{S}_a^{-1}\right)^{-1}$$

$\mathbf{S}_e$ is the error covariance matrix from measurements (random + correlated)

$\mathbf{S}_a$ is the error covariance matrix of the prior

$\hat{\mathbf{K}}$ is the Jacobian matrix



Primary iterations

Priors from ancillary data + initial guesses

TOA reflectance

Calculate the cost function χ^2

Update state vector

χ^2 converge?

No

Yes

Update Chl- a, γ

Calculate R_{rs}, Chl- a, γ

Chl- a, γ converge?

No

Yes

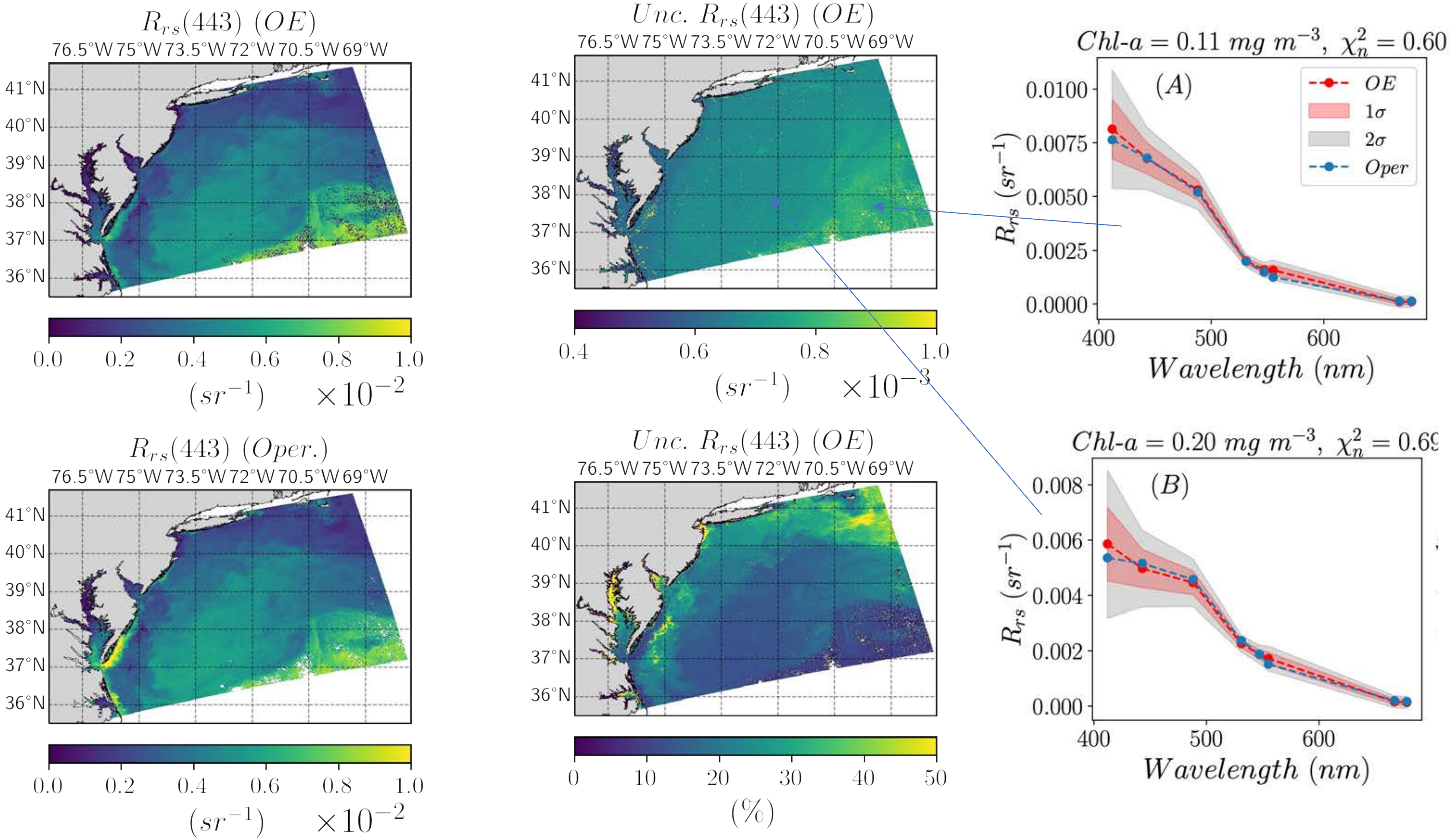
Calculate final R_{rs} and state vector

refinement iterations

Ibrahim et al. (2022)

Another type of algorithm to estimate the uncertainty

Bayesian OE algorithm test on real data (MODIS Aqua)



Ibrahim et al (2022)

Validating pixel-level uncertainty for the Bayesian algorithm

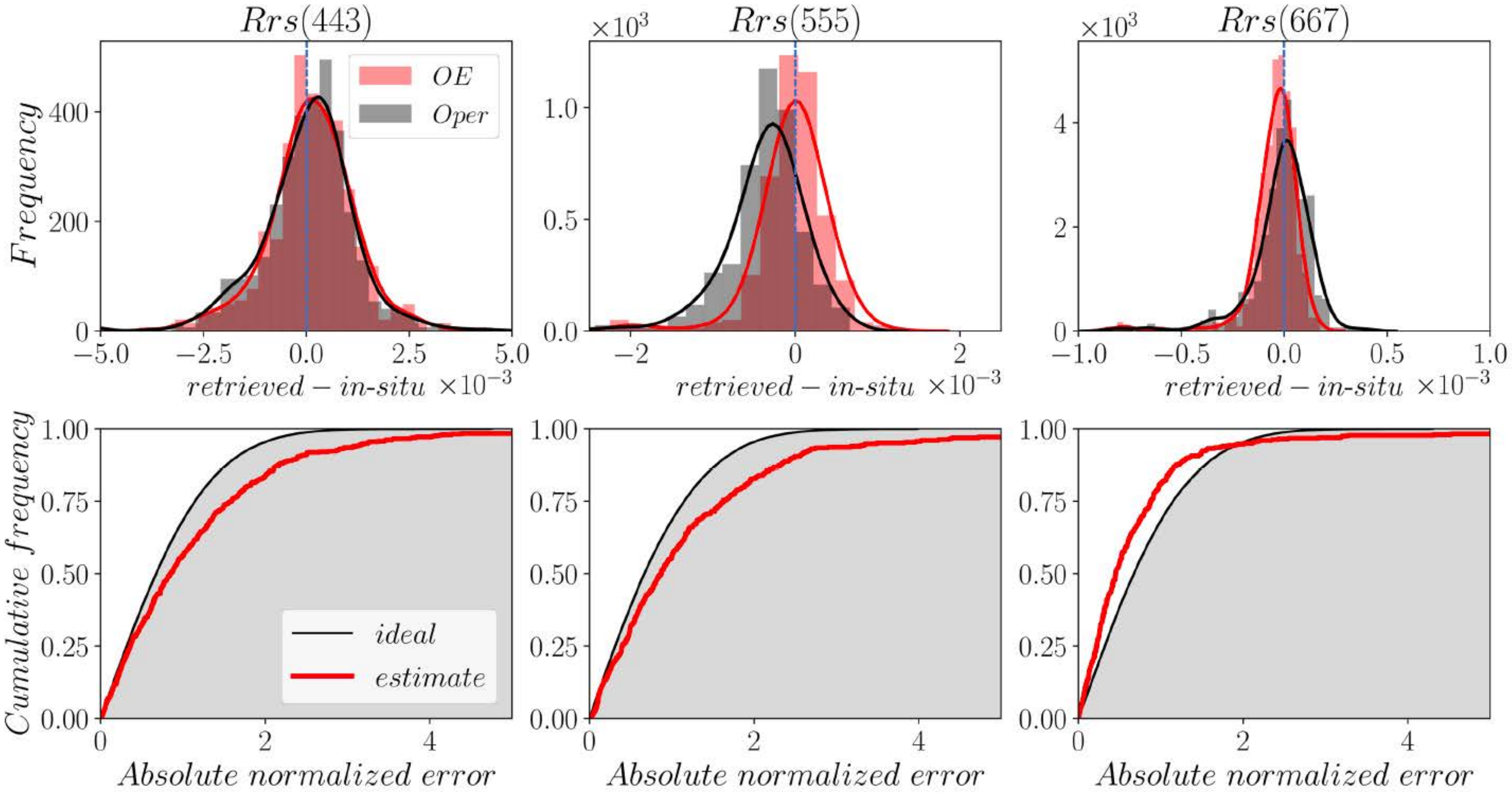


Fig. 7. Top row is a histogram of the difference between the retrieved and in-situ R_{rs} at 443, 555, and 667 nm, respectively, for the OE algorithm in red, and the operational algorithm in black. The bottom row is the CDF of the absolute normalized error Δ_N for R_{rs} at the same three bands, where the red curve is estimated from the OE algorithm, and the black curve is the ideal case for a standard normal.

Ibrahim et al (2022)

Questions?