Dynamic Error Estimates in GRASP: the assuring quality of the retrieved data

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GRASP error estimations in different applications:

- Retrieval of columnar properties of aerosol from the measurements by ground-based sun/sky-scanning radiometer alone;

AOD at 440, 675, 870 and 1020 nm and Sky radiances in solar almucantar from ±3.5 degrees to ±180 degrees

Herrera et al., 2022

Example: AERONET-like retrieval

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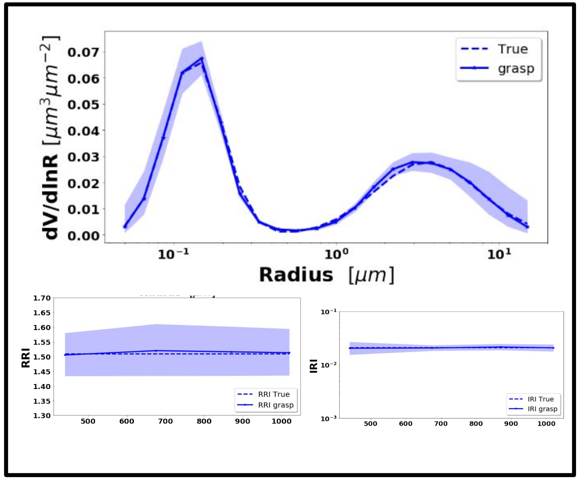
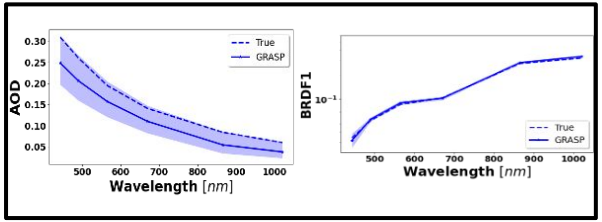


$$dV(r_i)/d\ln r_i,\ n(\lambda_i),\ k(\lambda_i),\ C_{sph} \text{ and } C_V(h)$$

- Aerosol and surface from the I, Q and U of POLDER/PARASOL observations.

GRASP/Components (size distribution as 5 bins simplification) simulated data: 2x2x30 pixels

Example: PARASOL-like retrieval



$$C_i,\ n(\lambda_i),\ k(\lambda_i),\ C_{sph},\ h,\ BRDF_{iso},\ BRDF_{vol},\ BRDF_{geom} \text{ and } BPDF$$

POLDER past polarimetric missions:

3MI/EPS-SG and MAP/CO2 polarimeters are to come in near future"

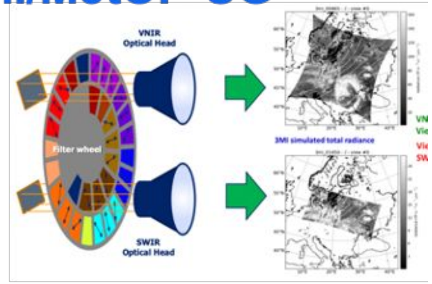
POLDER-1, -2, -3

08/1996- 06/1997

12/2003-09/2004

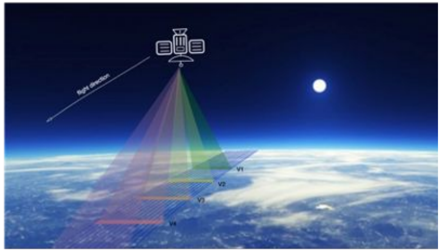
2004 - 2013

3MI/MetOP-SG

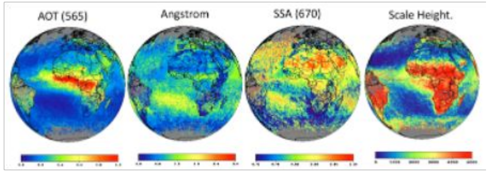


2026 - 2035

MAP/CO2M 2025



processed by GRASP



Aerosol L2 operational products of EUMETSAT to be based on GRASP algorithm

Multi-term LSM Solution in GRASP

$$\mathbf{f}_k^* = \mathbf{f}_k(\mathbf{a}) + \Delta\mathbf{f}_k^*$$

$$< \Delta\mathbf{f}_{k\,rand}^* >= \mathbf{0} \quad \text{and} \quad \mathbf{C}_{\mathbf{f}^*} = \begin{pmatrix} \mathbf{C}_1 & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{C}_2 & \mathbf{0} & \mathbf{0} \\ \dots & \dots & \dots & \dots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{C}_K \end{pmatrix}$$

Practical case:

$$\begin{cases} \mathbf{f}^* = \mathbf{f}^*(\mathbf{a}) + \Delta\mathbf{f}^* & \textit{measurements} \\ \mathbf{0}^* = \mathbf{S}_m + \Delta(\Delta^m \mathbf{a})^* & \textit{smoothness} \\ \mathbf{a}^* = \mathbf{a} + \Delta\mathbf{a}^* & \textit{a priori estimates} \end{cases}$$

$$\left(\sum_{k=1}^{K} \gamma_k \mathbf{K}_k^T (\mathbf{W}_k)^{-1} \mathbf{K}_k\right) \Delta\mathbf{a}^p = \sum_{k=1}^{K} \gamma_k \mathbf{K}_k^T (\mathbf{W}_k)^{-1} \Delta\mathbf{f}_k^p$$

Practical case:

$$\left(\mathbf{K}^T \mathbf{W}_f^{-1} \mathbf{K} + \gamma_a \mathbf{W}_a^{-1} + \gamma_g \Omega_m\right) \Delta\mathbf{a}^p =$$

$$= \mathbf{K}^T \mathbf{W}_f^{-1} \Delta\mathbf{f}^p + \gamma_a \mathbf{W}_a^{-1} (\mathbf{a}^p - \mathbf{a}^*) + \gamma_g \boldsymbol{\Omega}_m \mathbf{a}^p$$

measurement contribution

a priori contribution

Concept of dynamic error estimates in GRASP

- Based on rigorous statistical estimation approach
- A priori information is included using Multi-Term LSM (Least Square Method)
- Bias and input error variance estimated using **miss-fit of observations**

Dubovik et al., 2021
Herrera et al., 2022

$$\hat{\varepsilon}_0^2 \sim \frac{\Psi(\hat{\mathbf{a}}^p)}{(N_{meas} + N_{\mathbf{aprior}} - N_{\mathbf{a}})}$$

$$\begin{cases} \mathbf{C}_{\Delta\hat{\mathbf{a}}_{ran}} = \left((\mathbf{K}_p^T \mathbf{W}^{-1}\mathbf{K}_p) + \gamma_\Delta \Omega_m + \gamma_{\mathbf{a}^*}\mathbf{W}_{\mathbf{a}^*}^{-1}\right)^{-1}\hat{\varepsilon}_0^2 \\ \hat{\mathbf{a}}_{sys} = \left((\mathbf{K}_p^T\mathbf{W}^{-1}\mathbf{K}_p) + \gamma_\Delta\Omega_m + \gamma_{\mathbf{a}^*}\mathbf{W}_{\mathbf{a}^*}^{-1}\right)^{-1}\left(\mathbf{K}_p^T\mathbf{W}^{-1}\mathbf{b}_f + \gamma_\Delta\Omega_m\mathbf{b}_\Delta + \gamma_{\mathbf{a}^*}\mathbf{W}_{\mathbf{a}^*}^{-1}\mathbf{b}_{\mathbf{a}^*}\right) \end{cases}$$

Measurement contribution

A priori contribution

Basic concepts of formal propagation techniques

Example: Dynamic error estimates in GRASP

$$\hat{\mathbf{a}}_{estim} - \mathbf{a}_{real} = \Delta\hat{\mathbf{a}}_{ran} + \Delta\hat{\mathbf{a}}_{sys}$$

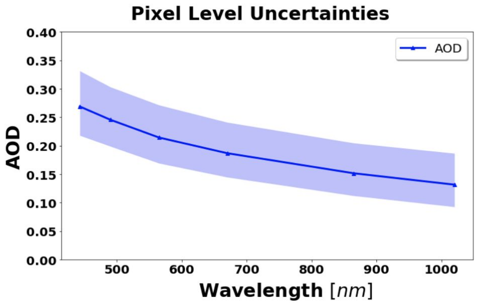
$$\underbrace{< \Delta\hat{\mathbf{a}}_{ran} >= 0}_{\textbf{random}} \qquad \underbrace{< \Delta\hat{\mathbf{a}}_{sys} >\neq 0}_{\textbf{systematic-bias}}$$

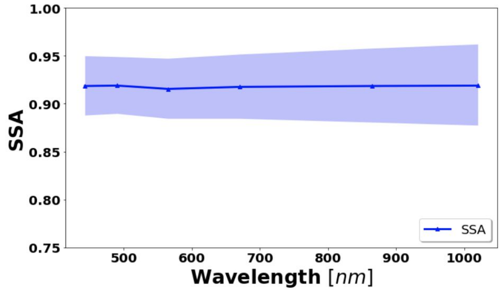
Dubovik et al., 2021
Herrera et al., 2022

$$\mathbf{C}_{\hat{\mathbf{a}}} = \left\langle (\Delta\hat{\mathbf{a}}_{ran} + \Delta\hat{\mathbf{a}}_{sys})(\Delta\hat{\mathbf{a}}_{ran} + \Delta\hat{\mathbf{a}}_{sys})^T \right\rangle = \mathbf{C}_{\Delta\hat{\mathbf{a}}_{ran}} + (\hat{\mathbf{a}}_{bias})(\hat{\mathbf{a}}_{bias})^T$$

$$Cov(\mathbf{a}) = \begin{pmatrix} \sigma_1^2 & \sigma_1\sigma_2\rho_{12} & \sigma_1\sigma_3\rho_{13} & \cdots \\ \sigma_2\sigma_1\rho_{21} & \sigma_2^2 & \sigma_2\sigma_3\rho_{23} & \cdots \\ \sigma_3\sigma_1\rho_{31} & \sigma_3\sigma_2\rho_{32} & \sigma_3^2 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$\pm\sigma_i$





$C_i,\ n(\lambda_i),\ k(\lambda_i),\ C_{sph},\ h,\ BRDF_{iso},\ BRDF_{vol},\ BRDF_{geom}$ and $BPDF$

Analysis of Non-diagonal elements of covariance matrix:

$$Cov(\mathbf{a}) = \begin{pmatrix} \sigma_1^2 & \sigma_1\sigma_2\rho_{12} & \sigma_1\sigma_3\rho_{13} & \cdots \\ \sigma_2\sigma_1\rho_{21} & \sigma_2^2 & \sigma_2\sigma_3\rho_{23} & \cdots \\ \sigma_3\sigma_1\rho_{31} & \sigma_3\sigma_2\rho_{32} & \sigma_3^2 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Correlation matrix

$$Corr(\mathbf{a}) = \begin{pmatrix} 1 & \rho_{12} & \rho_{13} & \cdots \\ \rho_{21} & 1 & \rho_{23} & \cdots \\ \rho_{31} & \rho_{32} & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

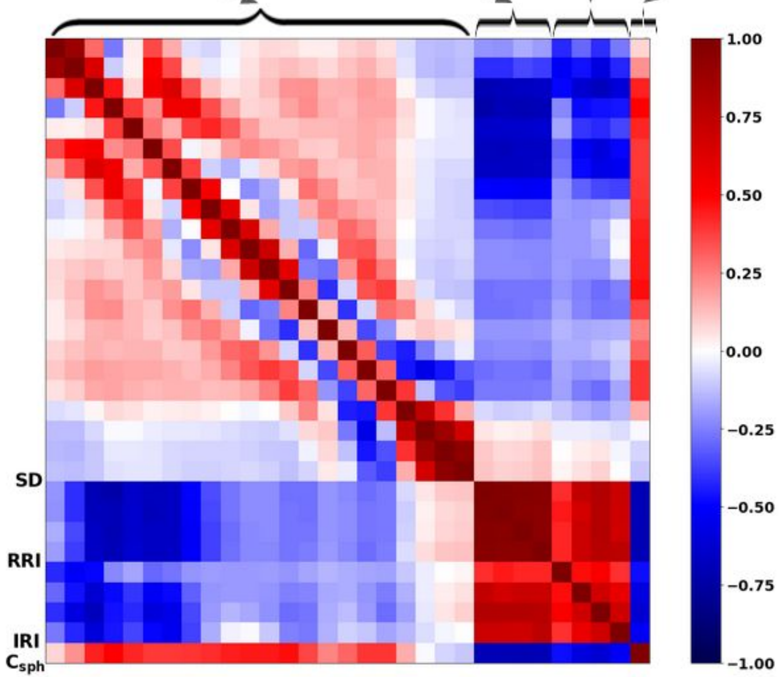
Some more details

Correlation matrix:

- Example for AERONET-like retrievals

$$\mathbf{a}^T = \left(\underbrace{\frac{dV}{dln(r_1)}, \cdots, \frac{dV}{dln(r_{22})}}; \underbrace{RRI_{\lambda_1}, \cdots, RRI_{\lambda_4}}; \underbrace{IRI_{\lambda_1}, \cdots, IRI_{\lambda_4}}; \underbrace{C_{sph}} \right)$$

$$Corr(\mathbf{a}) = \begin{pmatrix} 1 & \rho_{12} & \rho_{13} & \cdots \\ \rho_{21} & 1 & \rho_{23} & \cdots \\ \rho_{31} & \rho_{32} & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \longleftrightarrow$$

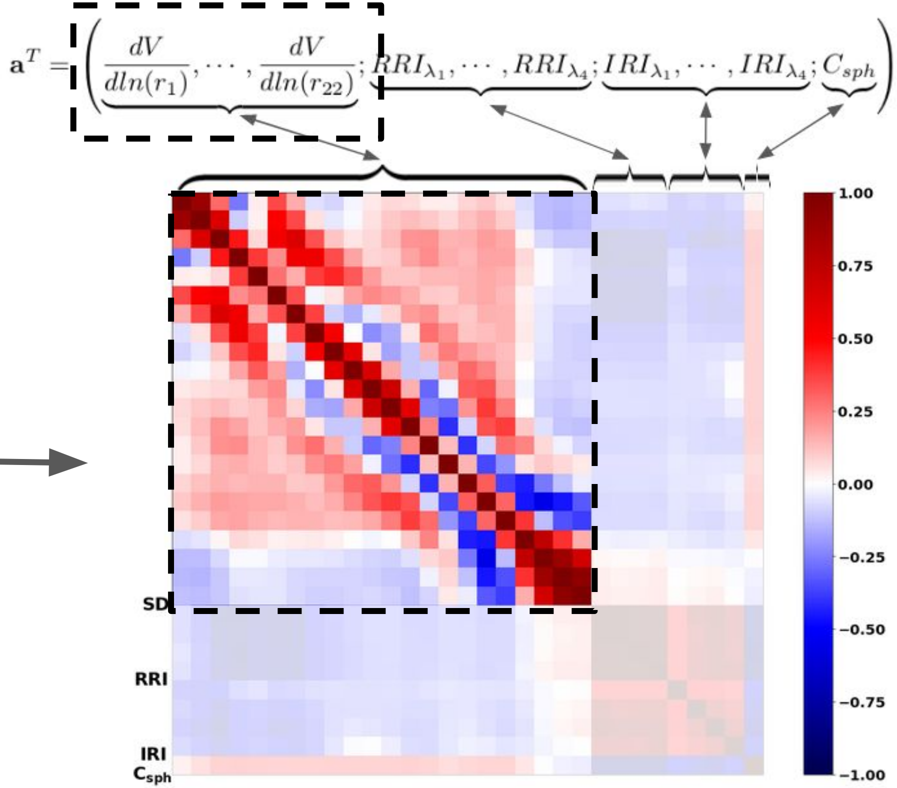


Herrera et al., 2022

Correlation matrix:

- Example for AERONET-like retrievals

$$Corr(\mathbf{a}) = \begin{pmatrix} 1 & \rho_{12} & \rho_{13} & \cdots \\ \rho_{21} & 1 & \rho_{23} & \cdots \\ \rho_{31} & \rho_{32} & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$



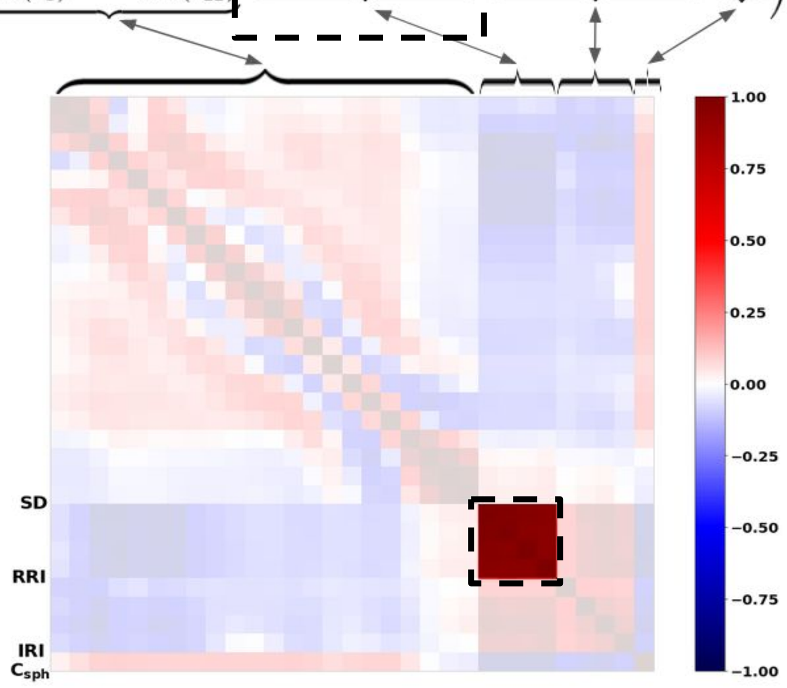
Herrera et al., 2022

Correlation matrix:

- Example for AERONET-like retrievals

$$Corr(\mathbf{a}) = \begin{pmatrix} 1 & \rho_{12} & \rho_{13} & \cdots \\ \rho_{21} & 1 & \rho_{23} & \cdots \\ \rho_{31} & \rho_{32} & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$\mathbf{a}^T = \left(\frac{dV}{dln(r_1)}, \cdots, \frac{dV}{dln(r_{22})}; RRI_{\lambda_1}, \cdots, RRI_{\lambda_4}; IRI_{\lambda_1}, \cdots, IRI_{\lambda_4}; C_{sph} \right)$$



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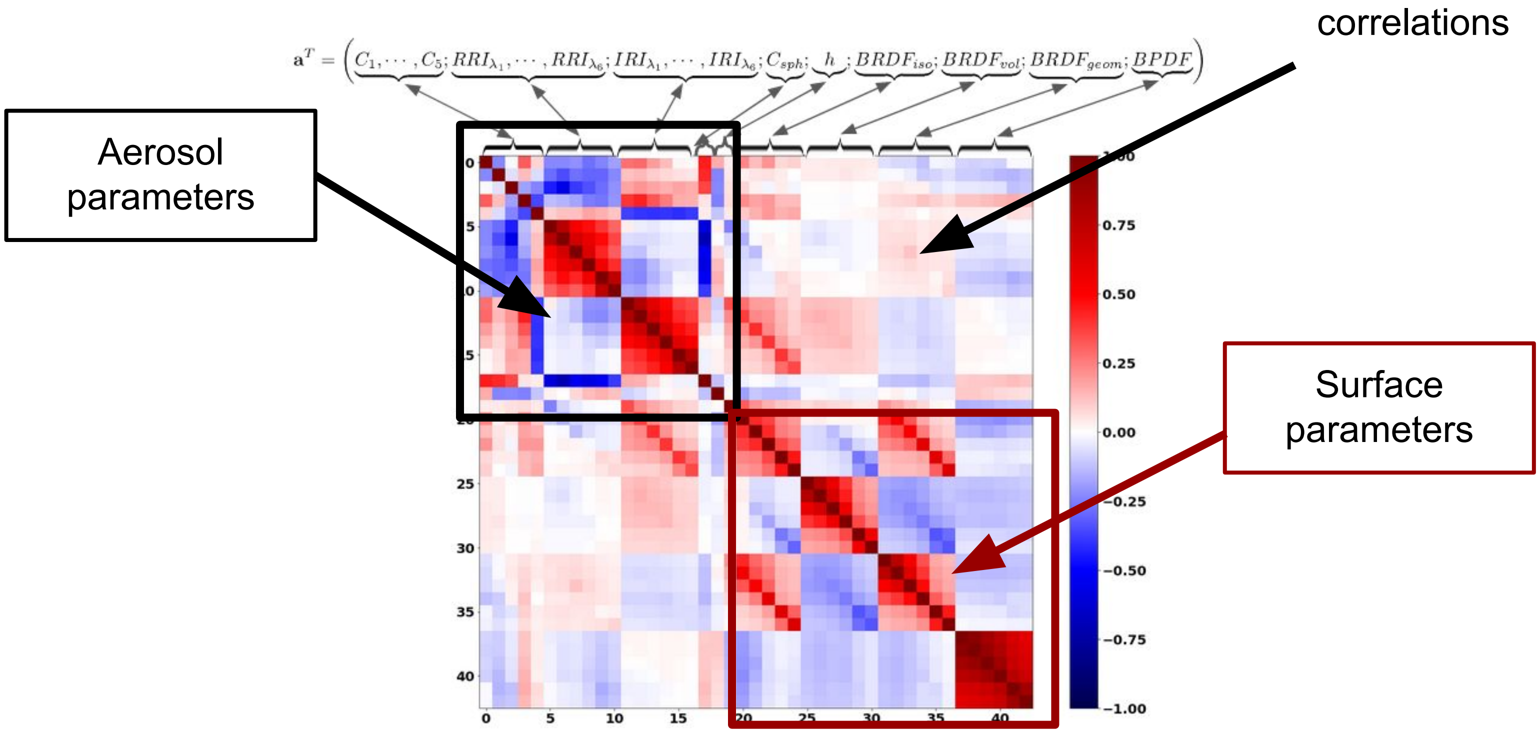
Correlation matrix:

- Example for POLDER/PARASOL-like retrievals



$$
\begin{cases}
\mathbf{C}_{\Delta\hat{\mathbf{a}}_{ran}} = \left(\left(\mathbf{K}_p^T \mathbf{W}^{-1} \mathbf{K}_p\right) + \gamma_\Delta \Omega_m + \gamma_{\mathbf{a}^*} \mathbf{W}_{\mathbf{a}^*}^{-1} \right)^{-1} \hat{\varepsilon}_0^2 \\
\hat{\mathbf{a}}_{sys} = \left(\left(\mathbf{K}_p^T \mathbf{W}^{-1} \mathbf{K}_p\right) + \gamma_\Delta \Omega_m + \gamma_{\mathbf{a}^*} \mathbf{W}_{\mathbf{a}^*}^{-1} \right)^{-1} \left(\left(\mathbf{K}_p^T \mathbf{W}^{-1} \mathbf{b}_f\right) + \gamma_\Delta \Omega_m \mathbf{b}_\Delta + \gamma_{\mathbf{a}^*} \mathbf{W}_{\mathbf{a}^*}^{-1} \mathbf{b}_{\mathbf{a}^*} \right)
\end{cases}
$$

Measurement contribution

A priori contribution

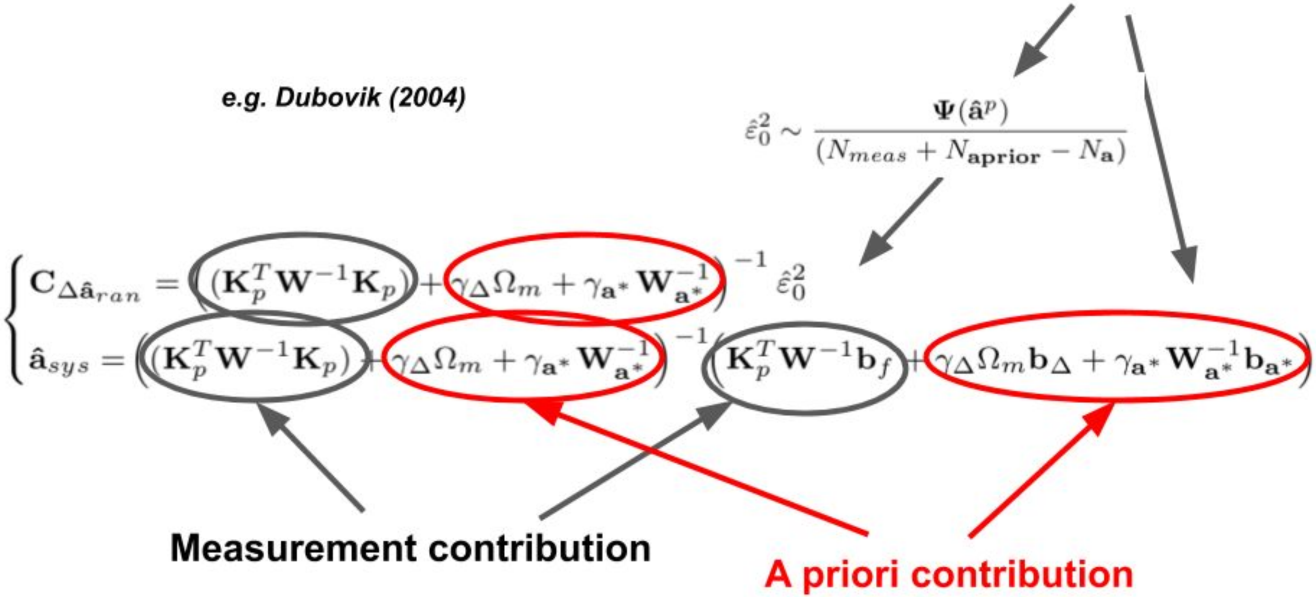
Errors for directly retrieved parameters:

$$
\begin{aligned}
\mathbf{C}_{\Delta\hat{m}} &\approx \mathbf{M}\left(\mathbf{C}_{\Delta\hat{\mathbf{a}}_{ran}} + \hat{\mathbf{a}}_{bias}\hat{\mathbf{a}}_{bias}^T\right)\mathbf{M}^T \\
&= \mathbf{M}\mathbf{C}_{\Delta\hat{\mathbf{a}}_{ran}}\mathbf{M}^T + \mathbf{M}\hat{\mathbf{a}}_{bias}(\mathbf{M}\hat{\mathbf{a}}_{bias})^T \\
&= \mathbf{C}_{\Delta\hat{m}_{ran}} + \hat{\mathbf{m}}_{bias}\hat{\mathbf{m}}_{bias}^T
\end{aligned}
$$

Errors for parameters that are functions of directly retrieved parameters

Improvements in Error Estimates by adding Bias in the calculations

- Bias and input error variance estimated using **miss-fit of observations**



$$\hat{\varepsilon}_0^2 \sim \frac{\Psi(\hat{\mathbf{a}}^p)}{(N_{meas} + N_{\mathbf{aprior}} - N_{\mathbf{a}})}$$

$$\begin{cases} \mathbf{C}_{\Delta\hat{\mathbf{a}}_{ran}} = \left((\mathbf{K}_p^T \mathbf{W}^{-1} \mathbf{K}_p) + \gamma_\Delta \Omega_m + \gamma_{\mathbf{a}^*} \mathbf{W}_{\mathbf{a}^*}^{-1} \right)^{-1} \hat{\varepsilon}_0^2 \\ \hat{\mathbf{a}}_{sys} = \left((\mathbf{K}_p^T \mathbf{W}^{-1} \mathbf{K}_p) + \gamma_\Delta \Omega_m + \gamma_{\mathbf{a}^*} \mathbf{W}_{\mathbf{a}^*}^{-1} \right)^{-1} \left(\mathbf{K}_p^T \mathbf{W}^{-1} \mathbf{b}_f + \gamma_\Delta \Omega_m \mathbf{b}_\Delta + \gamma_{\mathbf{a}^*} \mathbf{W}_{\mathbf{a}^*}^{-1} \mathbf{b}_{\mathbf{a}^*} \right) \end{cases}$$

Problem: Not all the bias can be seen in the miss-fit of observation

Improvements in Error Estimates by adding potential Bias

Proposed solution:

- We consider to include potential bias in the equation for systematic component

$$\hat{\mathbf{a}}^{\pm}_{bias} \approx \left(\mathbf{K}_p^T \mathbf{W}^{-1} \mathbf{K}_p\right)^{-1} \left(\mathbf{K}_p^T \mathbf{W}^{-1} (\mathbf{b}_f \pm \mathbf{b}_{bias})\right)$$

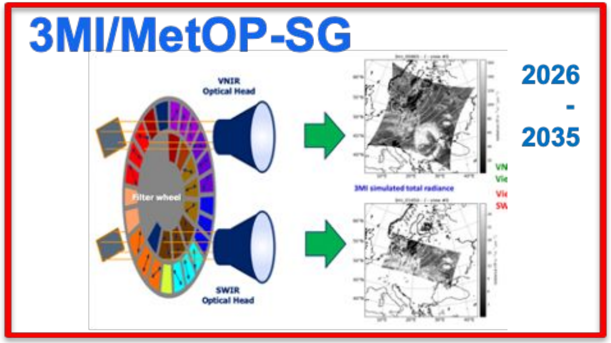
we assume three bias: **positive, negative and zero-bias**.

Added Biases:

PARASOL:

- Radiances +/- 0.5%
- Q, U components: +/- 0.001

Detailed evaluation of pixel level error estimates using a limited set of synthetic or proxy 3MI data



The diagonal elements of covariance matrix generated by **GRASP** for a key set of retrieved parameters (**AOD, AAOD, SSA, BRDF1**, etc.) was done.

- Sensitivity tests for synthetic data over Mongu and Banizoumbou at different noise level and biases
- Examples shown for bias and random noise added in measurements and systematic component: I 0.5% and for Q and U 0.001

Examples for simulated data over Mongu:

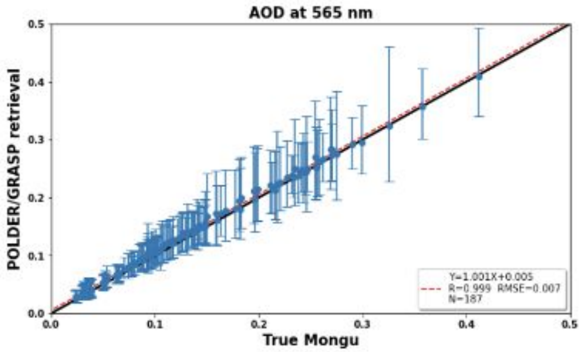
Improved approach

$$\sigma_{tot} = \sqrt{\sigma_{ran}^2 + \sigma_{bias}^2}$$

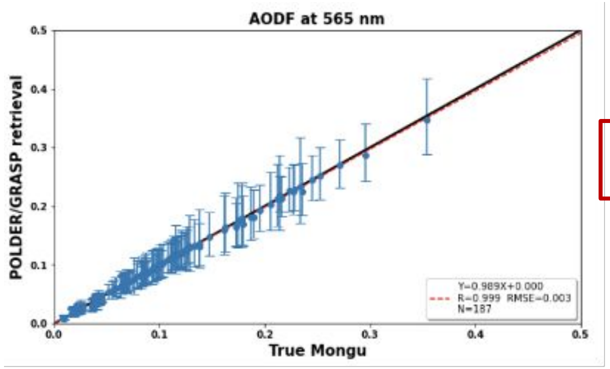
$$\sigma_{bias}^2 = \sigma_{lm}^2 + \sigma_{misfit}^2 + \frac{1}{N}\sum_{k=1}^{N}\sigma_k^2$$

- Bias and random noise added **in the measurements and in the systematic component**

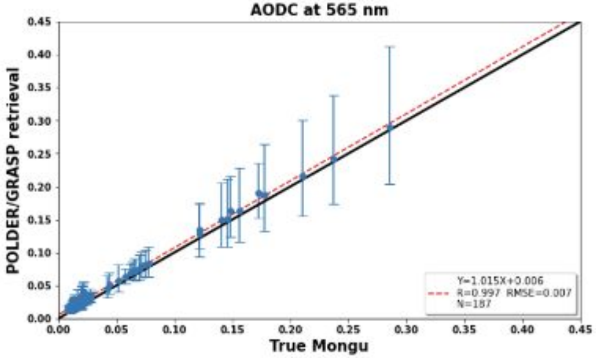
AOD



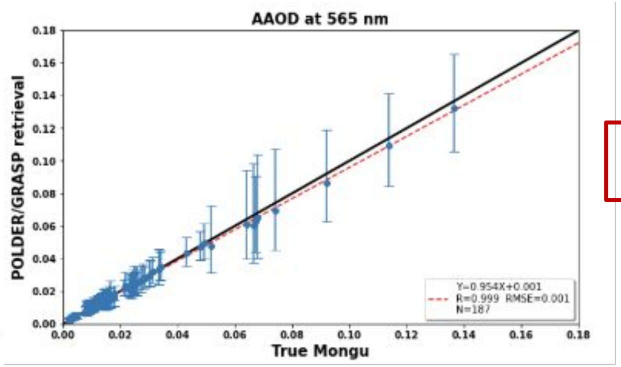
AODF



AODC



AAOD



Pixel level uncertainties

Examples for simulated data over Banizoumbou:

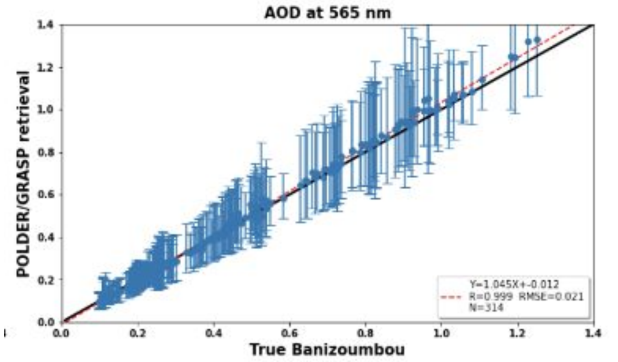
- Bias and random noise added **in the measurements and in the systematic component**

Improved approach

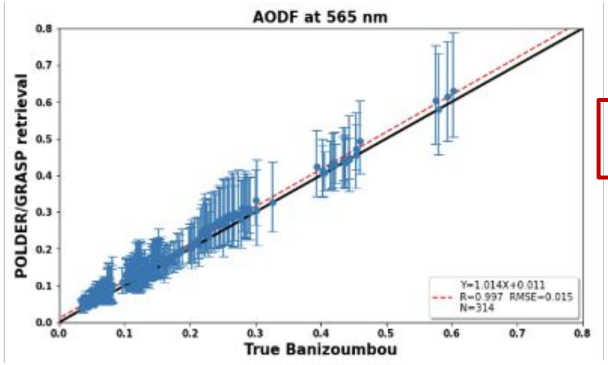
$$\sigma_{tot} = \sqrt{\sigma_{ran}^2 + \sigma_{bias}^2}$$

$$\sigma_{bias}^2 = \sigma_{lm}^2 + \sigma_{misfit}^2 + \frac{1}{N}\sum_{k=1}^{N}\sigma_k^2$$

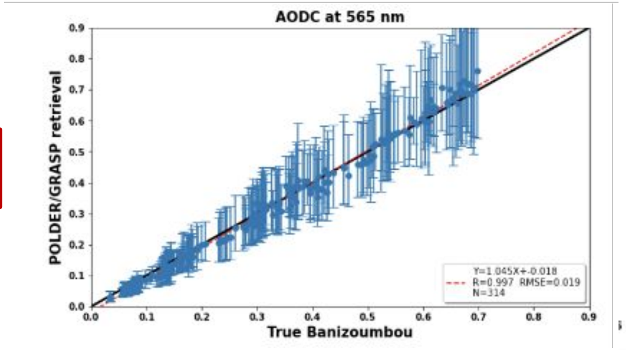
AOD



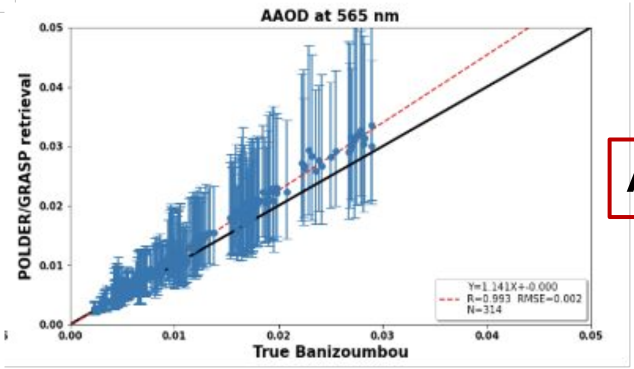
AODF



AODC



AAOD



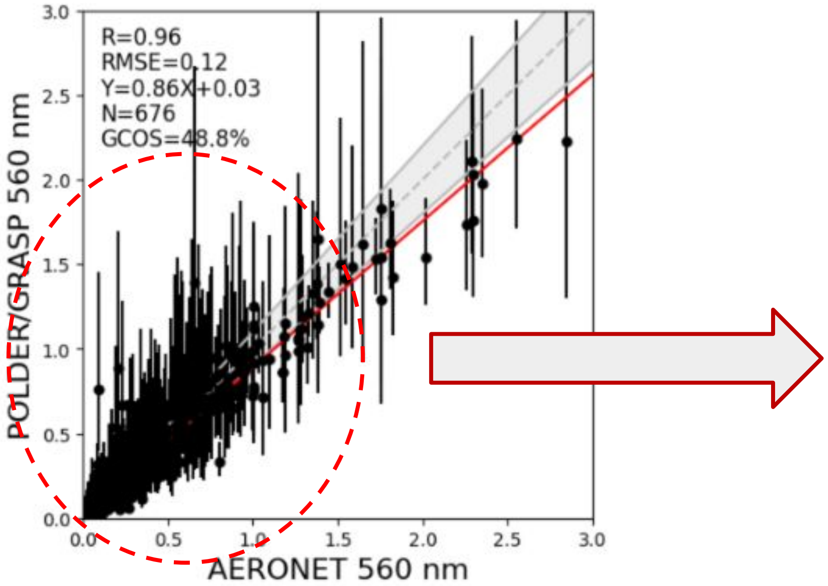
Pixel level uncertainties

Evaluation of pixel level error using an extensive data set of 3MI proxy data (e.g. POLDER) observations

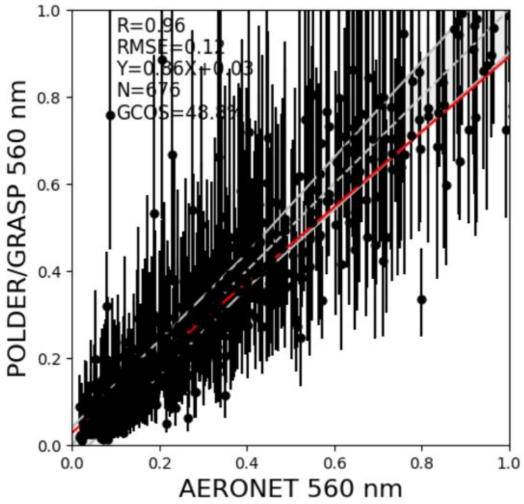
- Application in real data over 19 AERONET sites for the full 2008 year
- Bias added in the equation of the systematic component: I 0.5% and for Q and U 0.001

Quality criteria filter:

only based on the residual relative of 5%.



zoomed plot



Real applications:

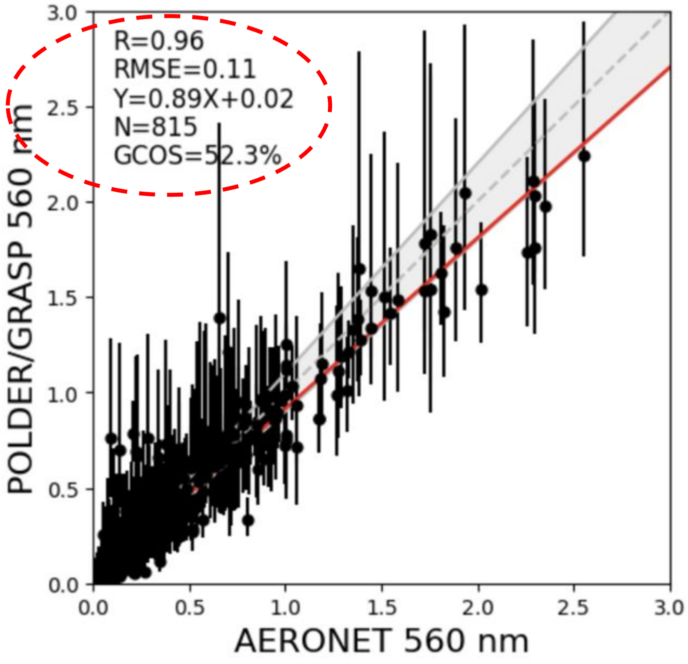
Improved approach

$$\sigma_{tot} = \sqrt{\sigma_{ran}^2 + \sigma_{bias}^2}$$

$$\sigma_{bias}^2 = \sigma_{lm}^2 + \sigma_{misfit}^2 + \frac{1}{N}\sum_{k=1}^{N}\sigma_k^2$$

- Example for POLDER/PARASOL retrievals over 19 AERONET sites

AOD



New Quality criteria filter:

absolute error varying according to the AOD

When AOD ≤ 0.6, the absolute error of AOD must be lower than 0.25.
When 0.6 < AOD ≤ 1.2, the absolute error of AOD must be lower than 0.5.
When 1.2 < AOD ≤ 3, the absolute error of AOD must be lower than 0.9.

Real applications:

- Example for POLDER/PARASOL retrievals over 19 AERONET sites

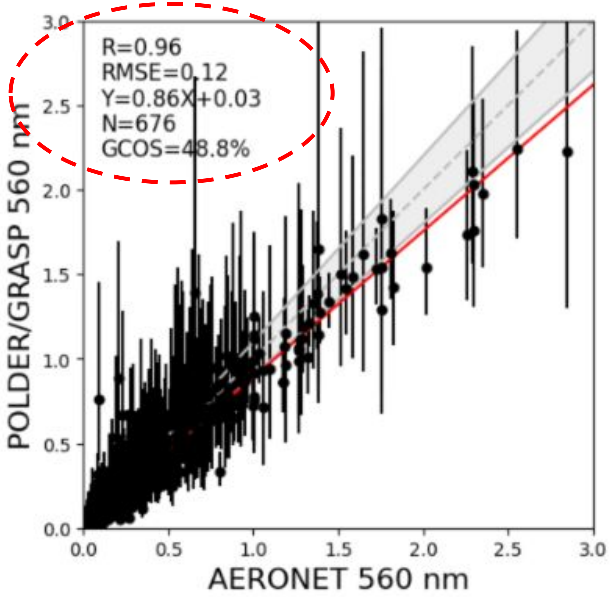
Improved approach

$$\sigma_{tot} = \sqrt{\sigma_{ran}^2 + \sigma_{bias}^2}$$

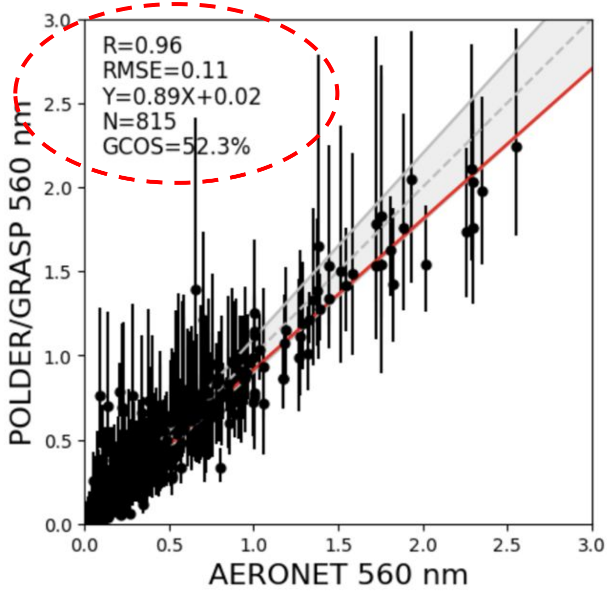
$$\sigma_{bias}^2 = \sigma_{lm}^2 + \sigma_{misfit}^2 + \frac{1}{N}\sum_{k=1}^{N}\sigma_k^2$$

AOD

Old criteria filter

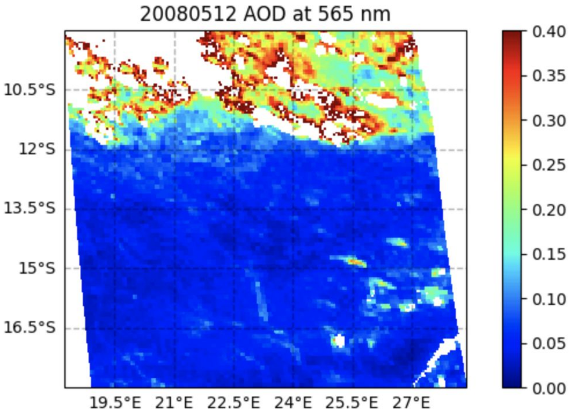


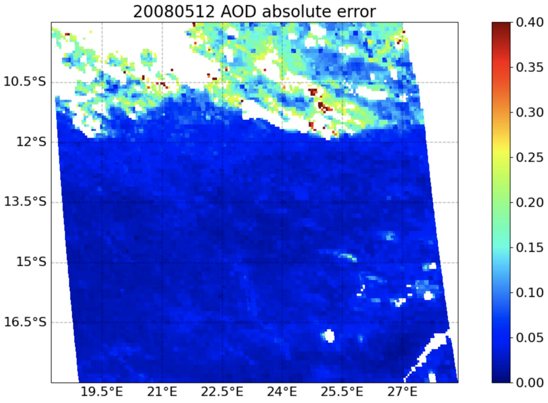
New criteria filter



Error images for POLDER data: Mongu

AOD

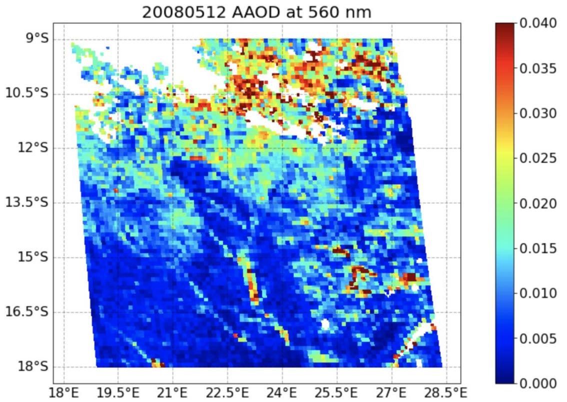


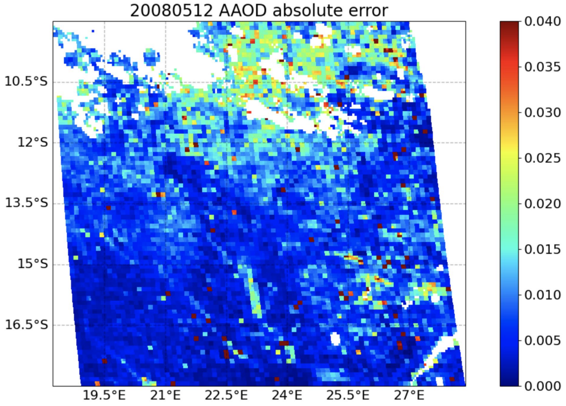


AOD absolute error

1000x1000km

AAOD



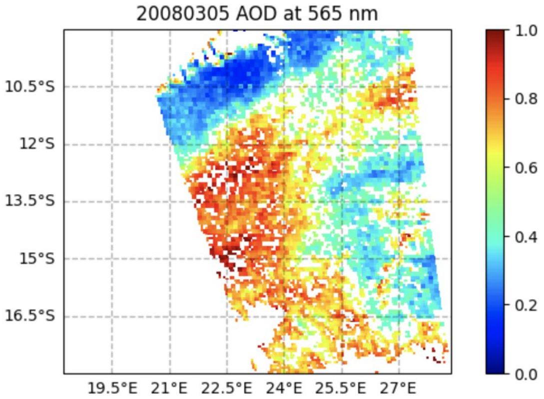


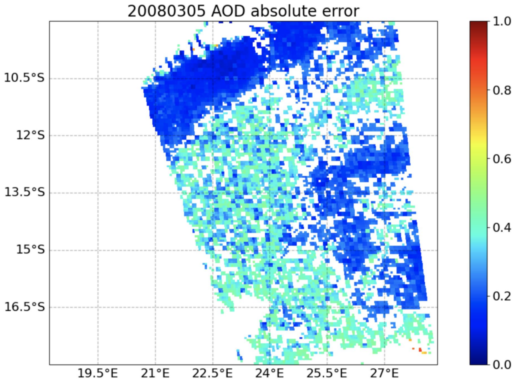
AAOD absolute error

Error images for POLDER data: Banizoumbou

AOD

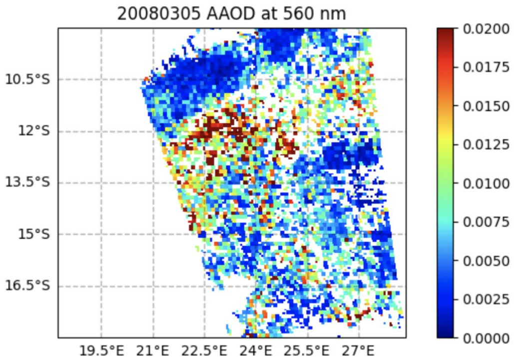
1000x1000km

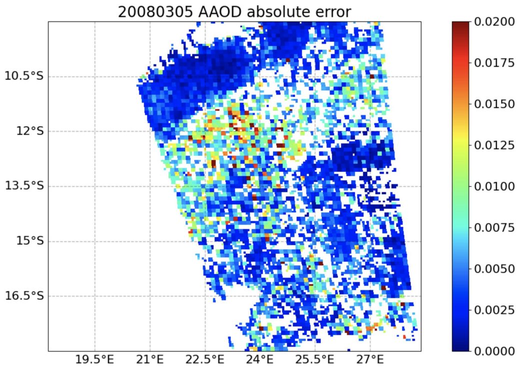




AOD absolute error

AAOD





AAOD absolute error

Summary

- The calculation of full covariance matrices for a key set of 3MI retrieved parameters was realized in **GRASP code**.

- The evaluation of diagonal elements of covariance matrix generated by **GRASP** for a key set of retrieved parameters (AOD, AAOD, SSA, BRDF1, etc.) was done.

- Several aspects were optimized for practical use of the pixel-level retrieval errors:
  - optimized accounting for systematic errors (bias);
  - the adjustments were introduced for the maximum values of obtained errors;

- The possibility of using the **GRASP** pixel-level retrieval errors **in product quality assurance criteria** were analyzed and demonstrated.