ALTIUS

L2 ozone retrieval algorithms

Didier Fussen, Noel Baker, Antonin Berthelot, Philippe Demoulin, Emmanuel Dekemper, Quentin Errera, Ghislain Franssens, Nina Mateshvili, Nuno Pereira, Didier Pieroux, Sotiris Sotiriadis

Belgian Institute for Space Aeronomy (BISA)

Contact: didier.fussen@oma.be

THE LIMB ....

ALTIUS

- RTM requirements: « fast », vectorial, spherical, refractive, 1 % accuracy ...
- LUT approach (convolved cross sections → convolved radiances)
- So far, Montecarlo methods were only considered as « slow » reference solutions.
- Then « **smartG** » came (HYGEOS)
  breaktrough: use massive power of GPU for parallelization: 1,5-5 millions ph/sec !

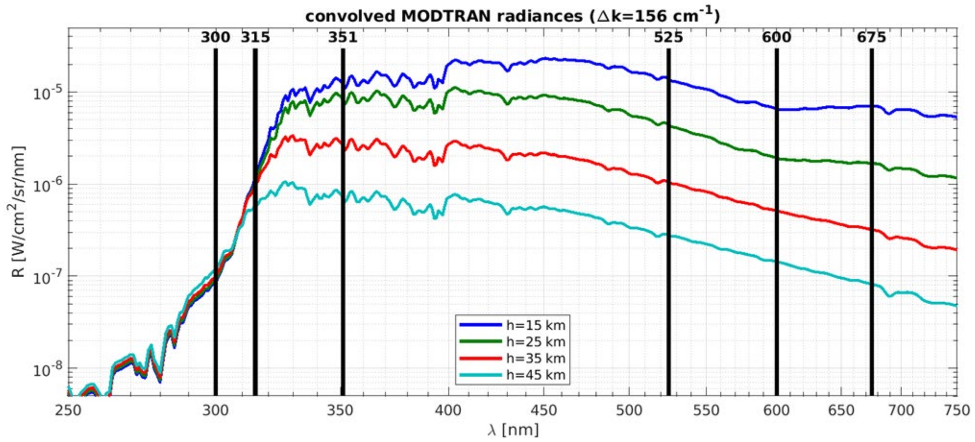
Systematic Comparison of Vectorial Spherical Radiative Transfer Models in Limb Scattering Geometry

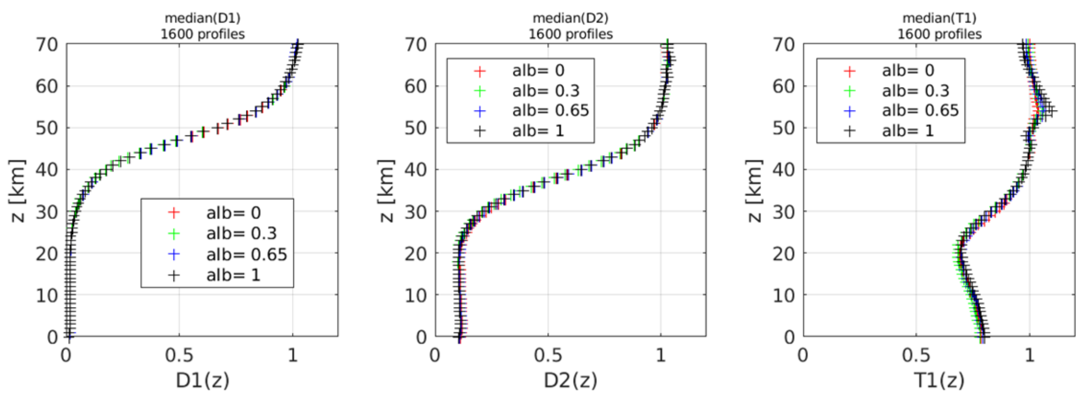
https://doi.org/10.5194/amt-2020-470

Daniel Zawada, Ghislain Franssens, Robert Loughman, Antti Mikkonen, Alexei Rozanov, Claudia Emde, Adam Bourassa, Seth Dueck, Hannakaisa Lindqvist, Didier Ramon, Vladimir Rozanov, Emmanuel Dekemper, Erkki Kyrölä, John P. Burrows, Didier Fussen, and Doug Degenstein

Model	Hardware Description	Time [minutes]	Scaled Runtime[a] [Minutes]
GSLS	Two Intel Xeon E5-2630 (6 physical cores at 2.3 GHz each)	35	13.0
SASKTRAN-HR	AMD 3900x (12 physical cores at 3.8 GHz)	7.4	7.4
SCIATRAN	Intel i7-6850 (6 physical cores at 3.6 GHz)	13.5	4.6
SASKTRAN-MC	AMD 3900x (12 physical cores at 3.8 GHz)	1909	1909
Siro	Four Intel Xeon E5-2630 (8 physical cores at 2.4 GHz each)	16560	20078
MYSTIC	AMD 3900x (12 physical cores at 3.8 GHz)	1906	1906
SMART-G	NVIDIA Titan V	59.2	N/A

Building a measurement vector
(vertical and spectral normalizations)





STATE VECTOR: 35 components

- up to 20 ozone PC
- up to 5 aerosol PC
- up to 5 air PC
- aerosol effective radius / PSD width
- albedo
- 2 solar angles

Every STOKES component (I,Q,U) is sampled at 31 altitudes (0:2:60 km)

The LUT-NN is a mapping 35 variables→ 31 observables

ALTIUS

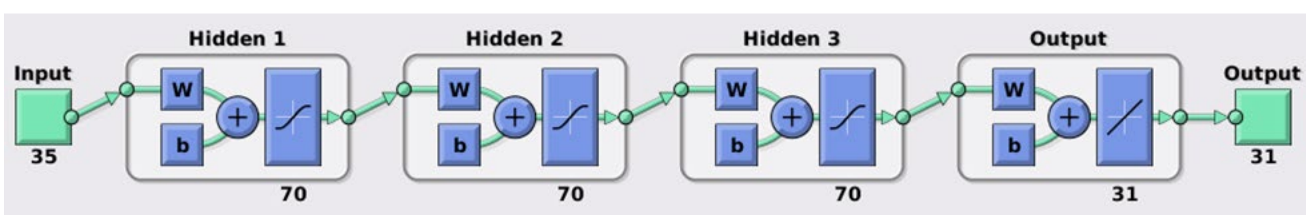
SUITLA 2.0

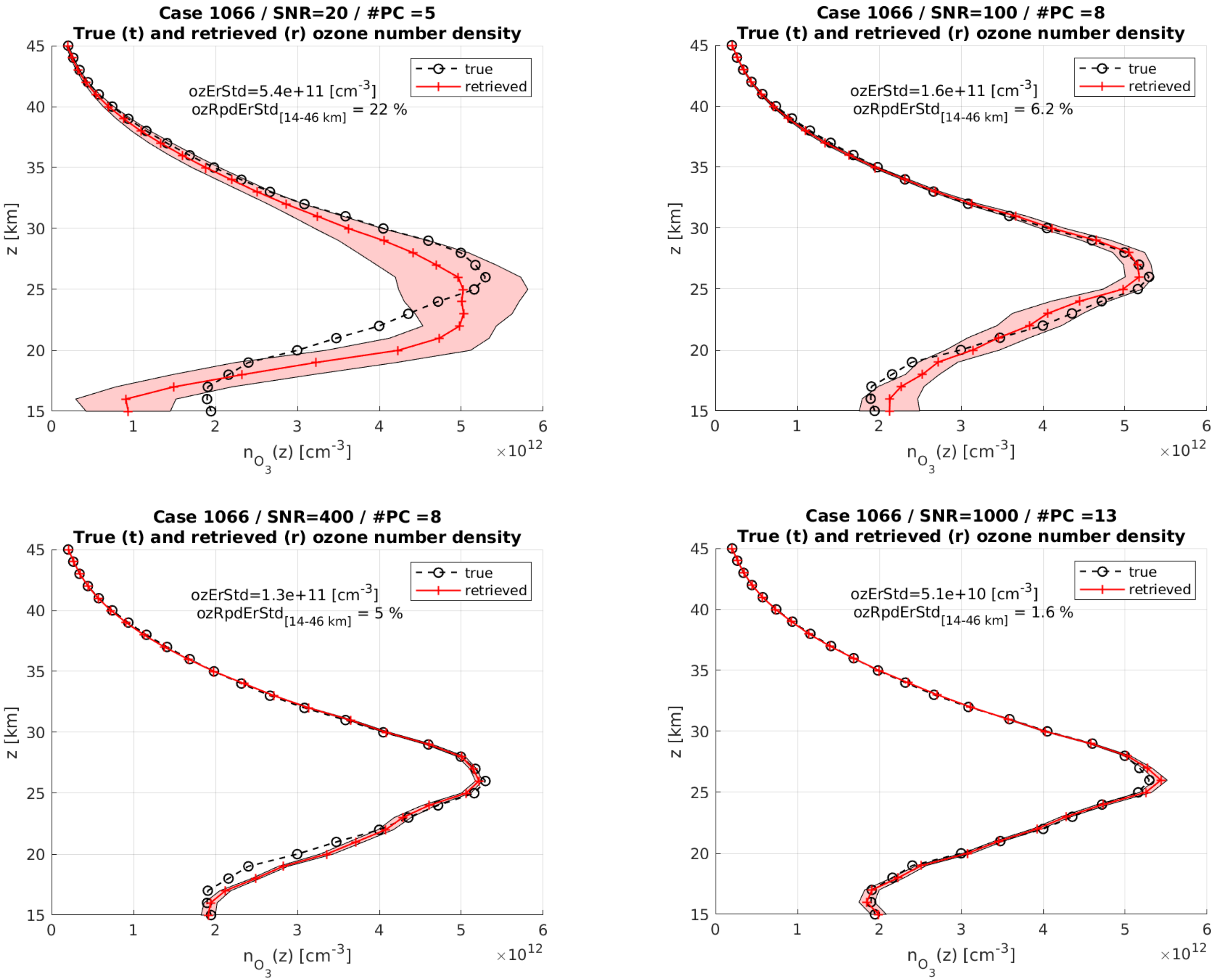
X_1	X_2	X_3	X_4	X_5	X_6	X_7	X_8	X_9	X_{10}
$a_{oz}(1)$	$a_{oz}(2)$	$a_{oz}(3)$	$a_{oz}(4)$	$a_{oz}(5)$	$a_{oz}(6)$	$a_{oz}(7)$	$a_{oz}(8)$	$a_{oz}(9)$	$a_{oz}(10)$
O_3	O_3	O_3	O_3	O_3	O_3	O_3	O_3	O_3	O_3

X_{11}	X_{12}	X_{13}	X_{14}	X_{15}	X_{16}	X_{17}	X_{18}	X_{19}	X_{20}
$a_{oz}(11)$	$a_{oz}(12)$	$a_{oz}(13)$	$a_{oz}(14)$	$a_{oz}(15)$	0	0	0	0	0
O_3	O_3	O_3	O_3	O_3	O_3	O_3	O_3	O_3	O_3

X_{21}	X_{22}	X_{23}	X_{24}	X_{25}	X_{26}	X_{27}	X_{28}	X_{29}	X_{30}
$a_{aer}(1)$	$a_{aer}(2)$	$a_{aer}(3)$	$a_{aer}(4)$	$a_{aer}(5)$	$a_{air}(1)$	$a_{air}(2)$	$a_{air}(3)$	0	0
n_{aer}	n_{aer}	n_{aer}	n_{aer}	n_{aer}	n_{air}	n_{air}	n_{air}	n_{air}	n_{air}

X_{31}	X_{32}	X_{33}	X_{34}	X_{35}	
r_e	σ	sza	saa	alb	
Effective radius	width	Sun zenith	Sun azimuth	albedo	




Case 1066 / SNR=20 / #PC =5
True (t) and retrieved (r) ozone number density
true
retrieved
ozErStd=5.4e+11 [cm-3]
ozRpdErStd[14-46 km] = 22 %
z [km]
n_O3(z) [cm-3]
×10^12
Case 1066 / SNR=100 / #PC =8
True (t) and retrieved (r) ozone number density
true
retrieved
ozErStd=1.6e+11 [cm-3]
ozRpdErStd[14-46 km] = 6.2 %
z [km]
n_O3(z) [cm-3]
×10^12
Case 1066 / SNR=400 / #PC =8
True (t) and retrieved (r) ozone number density
true
retrieved
ozErStd=1.3e+11 [cm-3]
ozRpdErStd[14-46 km] = 5 %
z [km]
n_O3(z) [cm-3]
×10^12
Case 1066 / SNR=1000 / #PC =13
True (t) and retrieved (r) ozone number density
true
retrieved
ozErStd=5.1e+10 [cm-3]
ozRpdErStd[14-46 km] = 1.6 %
z [km]
n_O3(z) [cm-3]
×10^12

Reduced Chi-squared strategy

$$\chi^2 = \sum_{n=1}^{N} \left(\frac{y_n - f(\vec{x}_n; \vec{\theta})}{\sigma_n} \right)^2$$

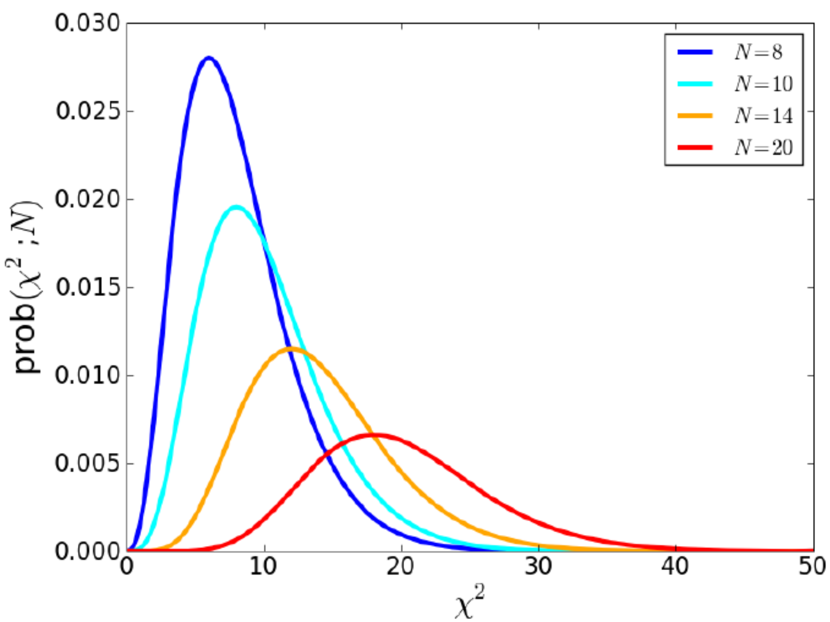
$$\chi^2_{\rm red} = \frac{\chi^2}{K}$$

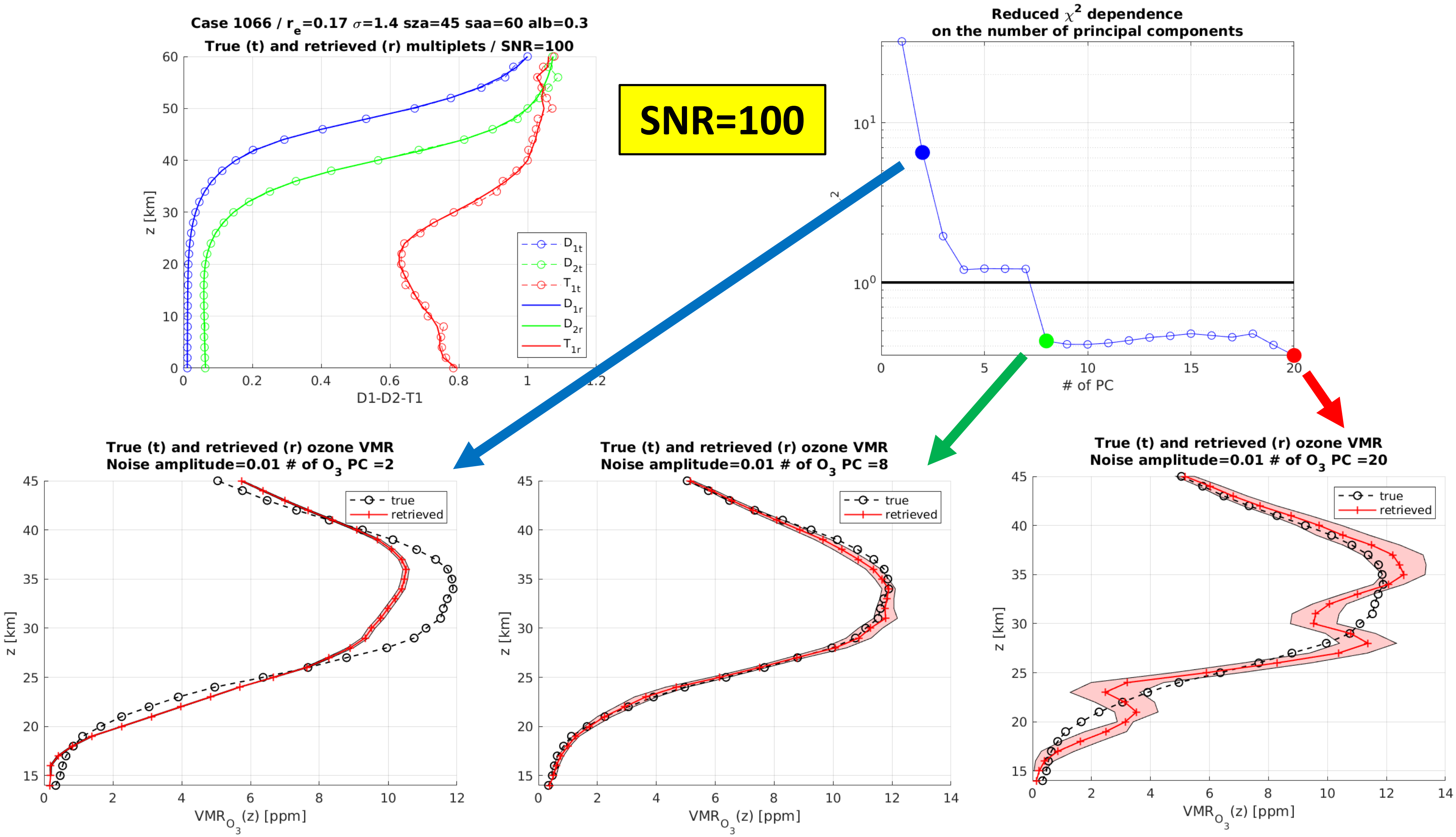
K=N-P **if and only if** the P parameters are independent→ property of PCA!

$$\text{prob}(\chi^2; K) = \frac{1}{2^{K/2}\Gamma(K/2)} \left(\chi^2\right)^{K/2-1} e^{-\chi^2/2}$$

$$\langle \chi^2 \rangle = \int_0^\infty \chi^2 \, \text{prob}(\chi^2; K) \, d\chi^2 = K$$

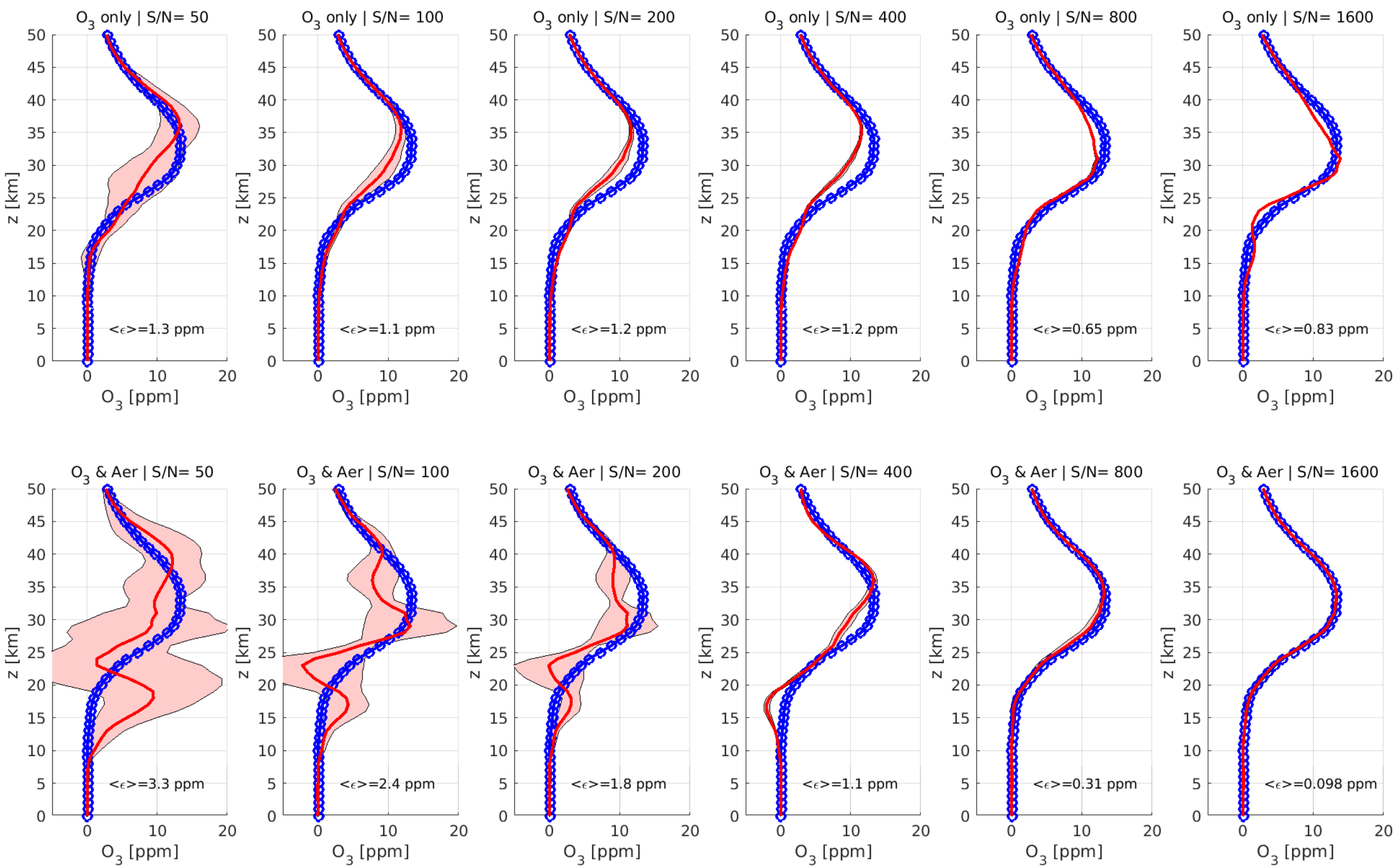
IF WE VARY P, TARGET IS $\chi^2_{\rm red} = \frac{\chi^2}{K}$ **≅ 1**





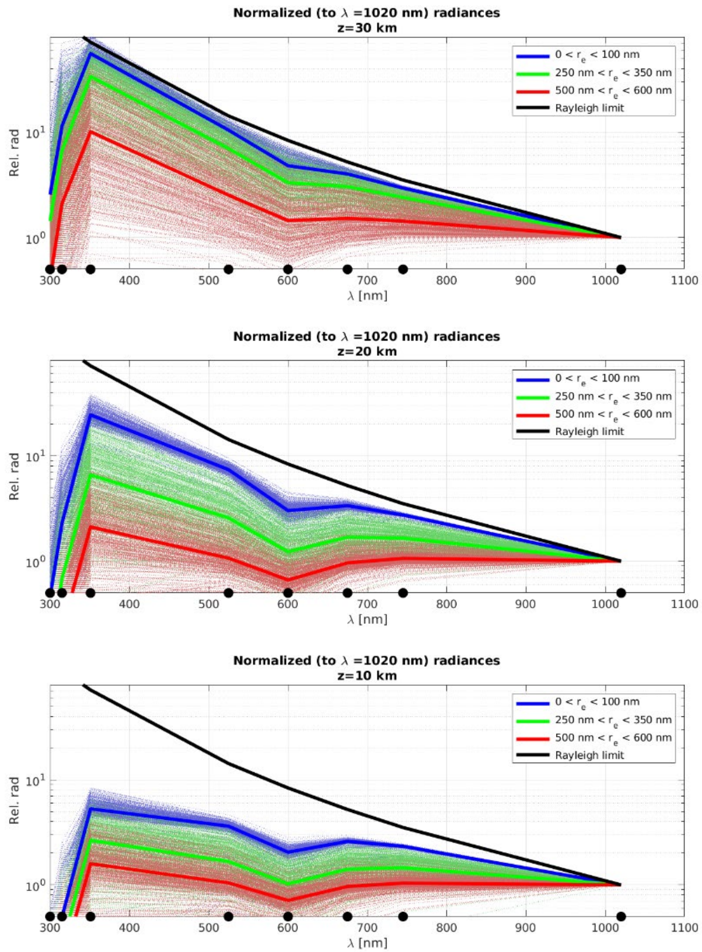
Case 1066 / r_e=0.17 σ=1.4 sza=45 saa=60 alb=0.3
True (t) and retrieved (r) multiplets / SNR=100
z [km]
D1-D2-T1
D_{1t}
D_{2t}
T_{1t}
D_{1r}
D_{2r}
T_{1r}
SNR=100
Reduced χ^2 dependence
on the number of principal components
# of PC
True (t) and retrieved (r) ozone VMR
Noise amplitude=0.01 # of O_3 PC =2
true
retrieved
VMR_{O_3}(z) [ppm]
True (t) and retrieved (r) ozone VMR
Noise amplitude=0.01 # of O_3 PC =8
True (t) and retrieved (r) ozone VMR
Noise amplitude=0.01 # of O_3 PC =20

How SNR is the driver… Aerosol retrieval improves ozone IF SNR ≥ 500

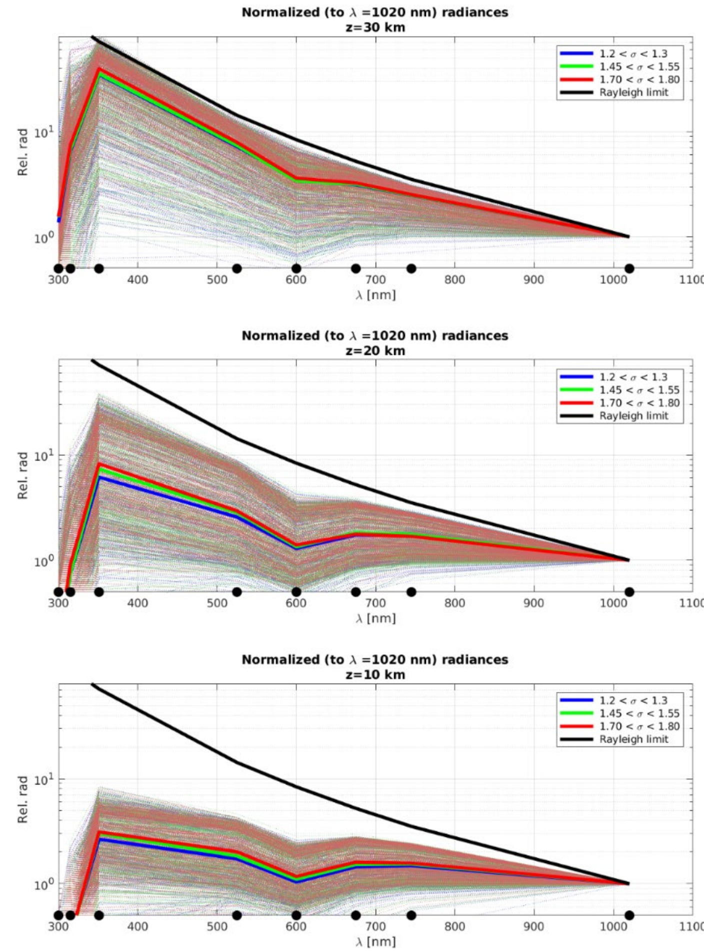


The preferred approach for ozone NRT is a **perturbative ("step-by-step") inversion** where aerosols, albedo are independently derived and frozen during ozone retrieval (inner loop). In the consolidated phase, this process is iterated (outer loop)

The impact of the aerosol spectral properties on the ozone error budget

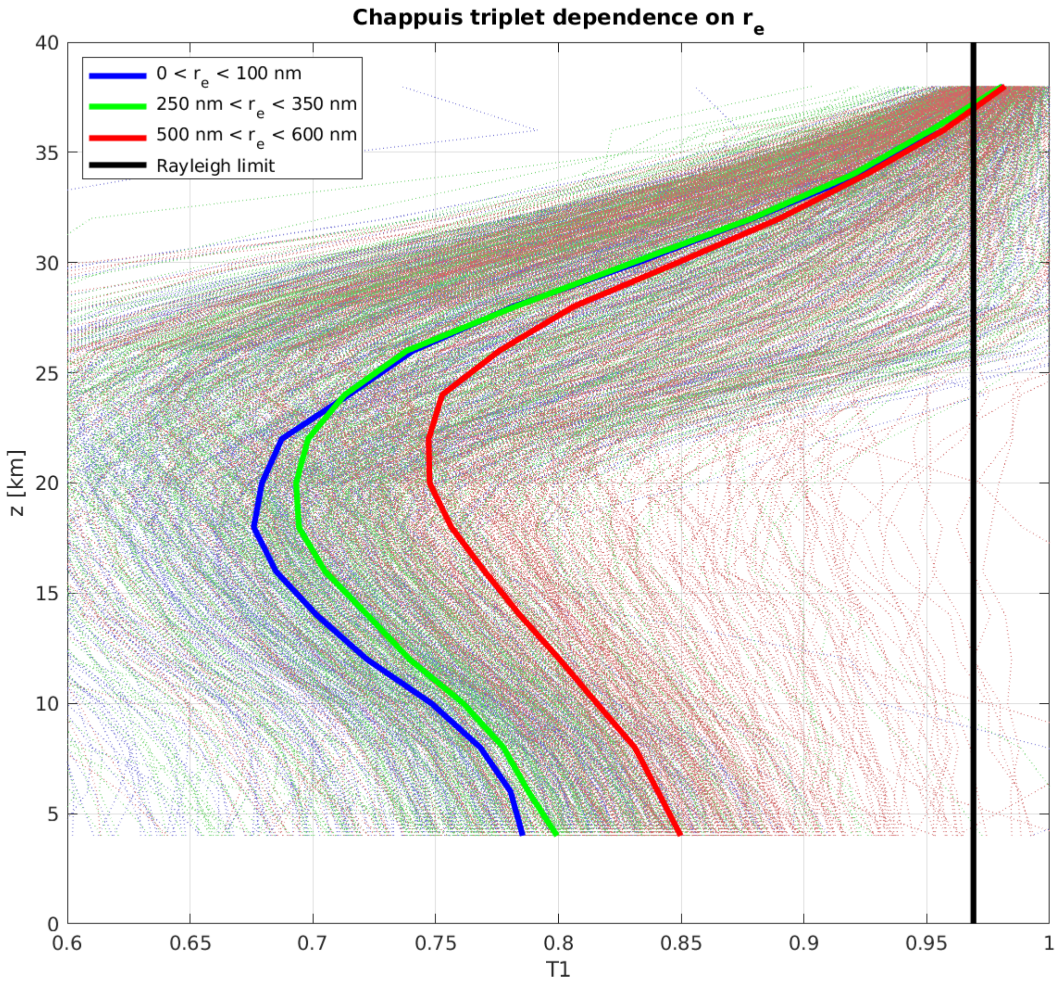


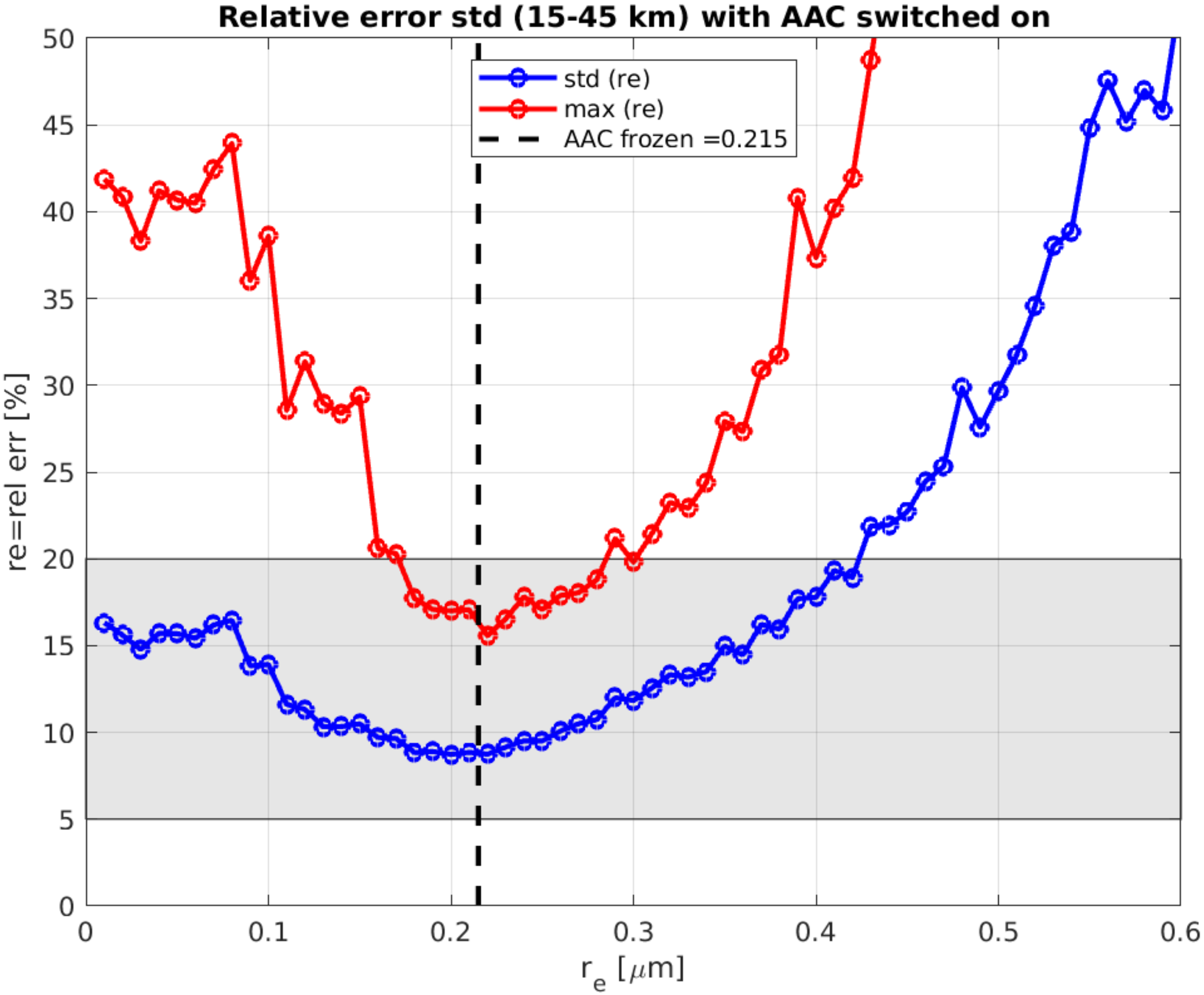
r_e

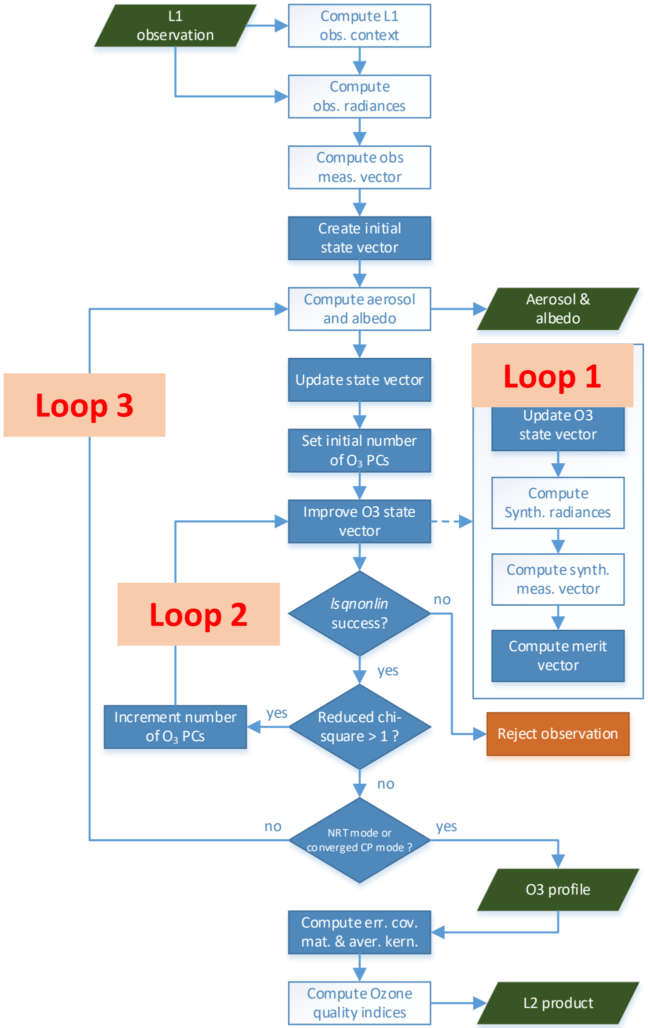


σ

The « triplet » profile is the primary source of ozone information content in the lower stratosphere.




Relative error std (15-45 km) with AAC switched on
std (re)
max (re)
AAC frozen =0.215
re=rel err [%]
r_e [μm]
0
5
10
15
20
25
30
35
40
45
50
0
0.1
0.2
0.3
0.4
0.5
0.6



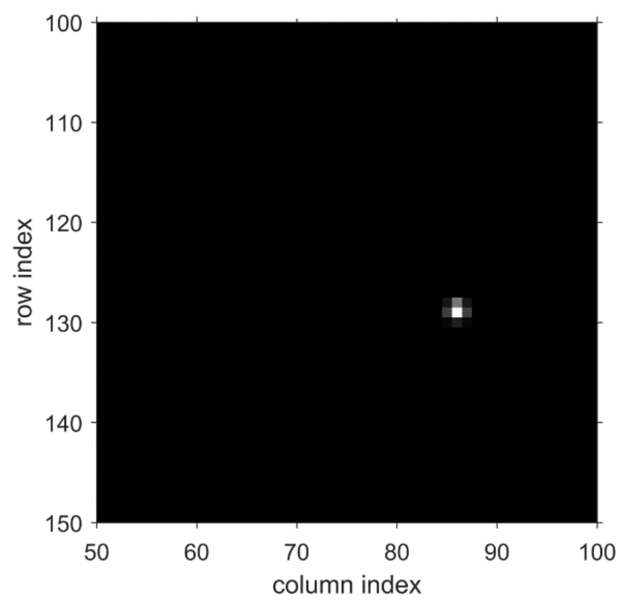
ALTIUS limb ozone retrieval today

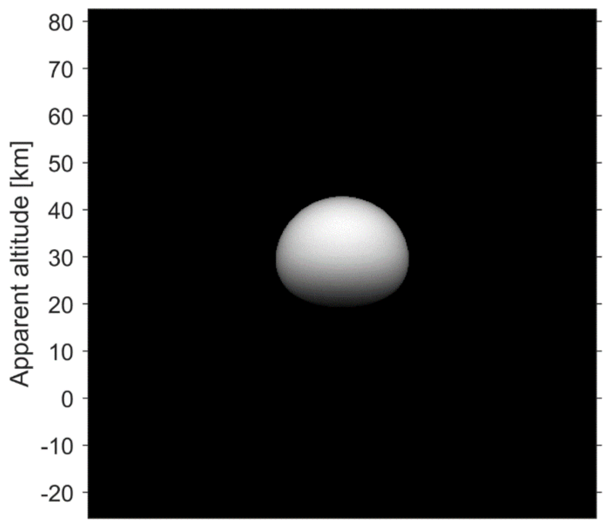
- [NRT] loop 1: # of PC is set to P; standard optimization of the weighted squared differences between observed and computed multiplets (Matlab « trust region» or L-M algorithm); $\chi^2_r(P)$ is computed @ the solution.
- [NRT] loop 2: the state vector resolution is incremented (P→P+1), starting from the P-solution , till reduced $\chi^2_r(P+1) \cong 1$
- [CP] loop 3: aerosol and albedo are updated + fine tuning of side effects (spectral convolutions, residual straylight, ECMWF analyses,..etc)

Stellar/planetary/lunar/solar occultations

ALTIUS will perform stellar, planetary, solar, and lunar occultations at each orbit, enabling the measurement of atmospheric transmittance profiles at selected wavelengths.

	Typical stellar/planetary occultation	Typical solar/lunar occultation
Acquisition wavelengths [nm]	310, 320, 442, 603, 1020	310, 320, 442, 603, 1020
Exposure time [s]	0,5	0,1
Occultation duration [s]	60-90	70
TP altitude range [km]	20-115	10-115
# images acquired	~300	~1200





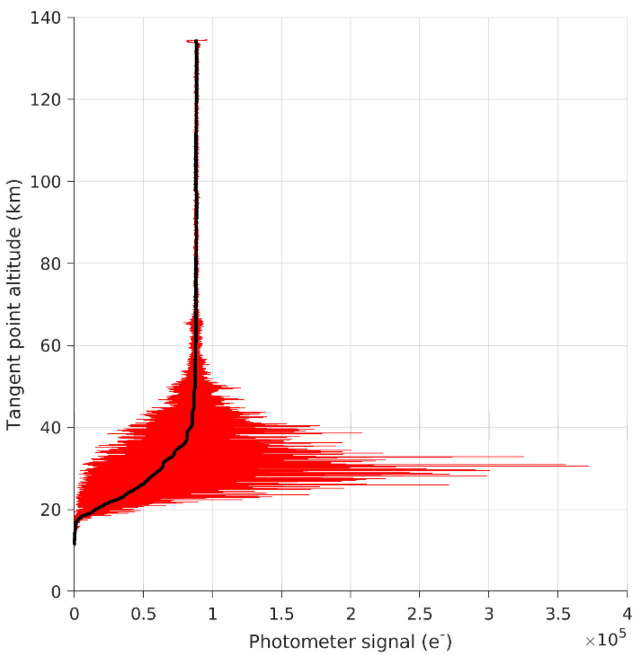
Stellar/planetary/lunar/solar occultations

The O_3 **retrieval algorithm** is a non-linear χ^2 minimization with Levenberg-Marquardt damping and Tikhonov regularization (both distance to a priori profile, and profile smoothness have been tested).

Particular aspects:

- The O_3 profile is described by an **expansion on up to 25 orthogonal functions** (same principal components as the limb chain).
- The measurement vector consists of **ratios of transmittance profiles** to mitigate scintillation, and aerosol interference.
- The forward model **Jacobian is analytical**.

	state vector	measurement vector
O_3	linear, scaled PCA (25 PC) $x = (c_1, \dots, c_{25})^t$	$y = (d_1, d_2, d_3)^t$, with $d_1 = \frac{t_{310}}{t_{442}}, d_2 = \frac{t_{320}}{t_{442}}, d_3 = \frac{t_{603}}{t_{750}}$



Approach for **mitigating the star dilution and scintillation**: division of simultaneously measured transmittances

Transmittance signal: $T_{atm}(\lambda, t) \approx T_{ext}(\lambda, t) \times T_d(t) \times T_{sc}(t)$

Ratio of concurrent transmittance measurements at 2 wavelengths:

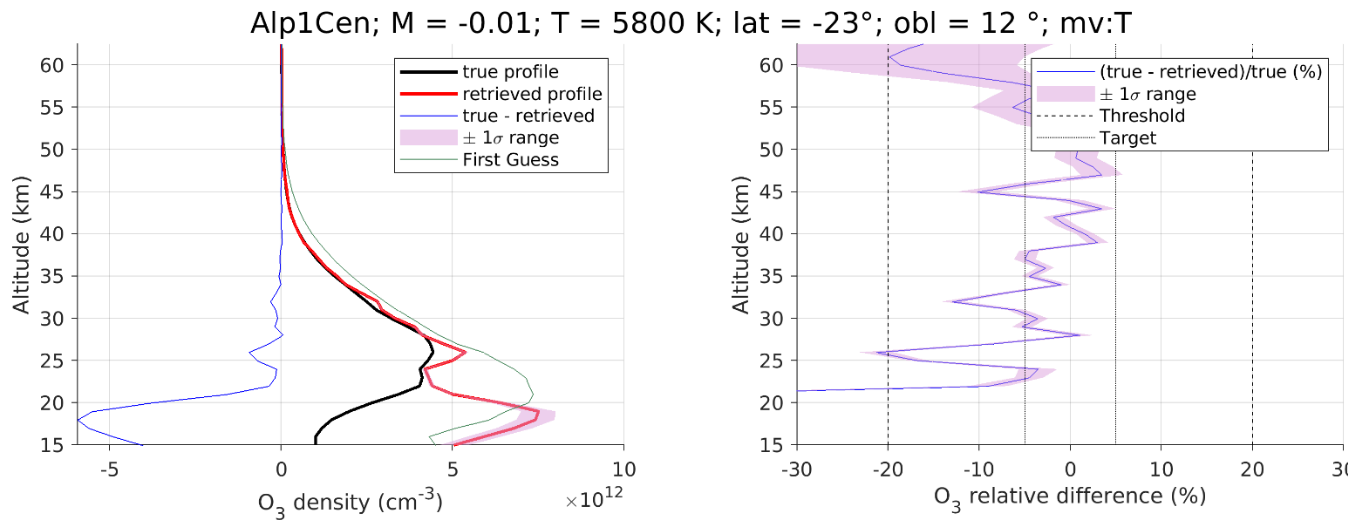
$$\frac{T_{atm}(\lambda_1, t)}{T_{atm}(\lambda_2, t)} \approx \frac{T_{ext}(\lambda_1, t)}{T_{ext}(\lambda_2, t)} = e^{-(\tau(\lambda_1, t) + \tau(\lambda_2, t))}$$

Stellar/planetary/lunar/solar occultations

The O_3 retrieval algorithm has been applied to genuine **GOMOS L1 data**. The main objective is to quantify how well the scintillation mitigation works.

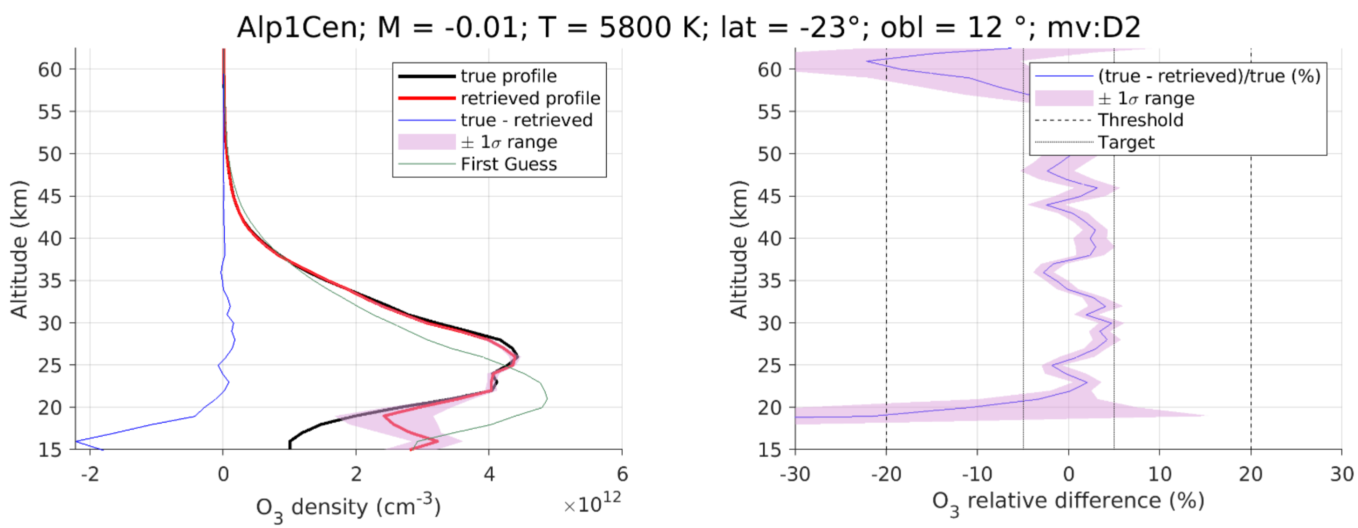
Without scintillation mitigation

(the measurement vector is made of simple transmittance profiles)



With scintillation mitigation

(the measurement vector is made of ratios of simultaneously measured spectral transmittances)

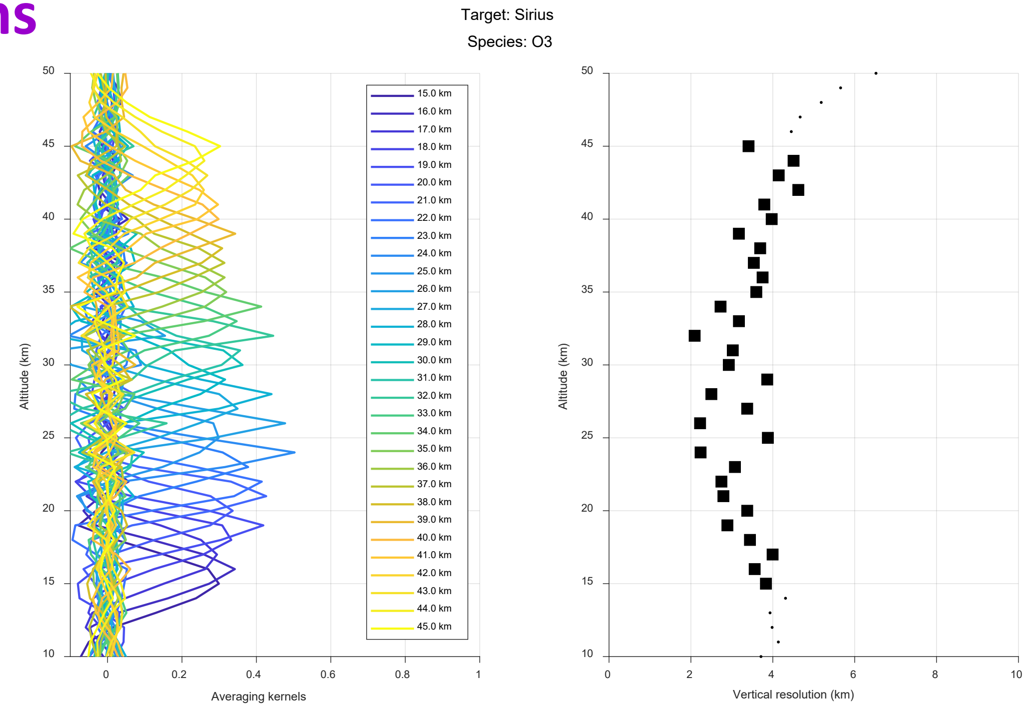


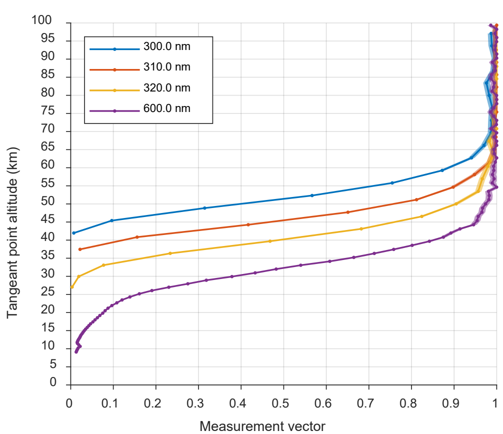
Stellar/planetary occultations

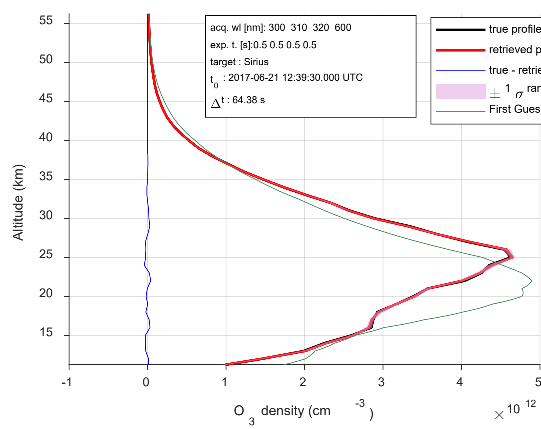
The global retrieval algorithm fits the O_3 profile to the measured transmittance profiles at selected wavelengths.

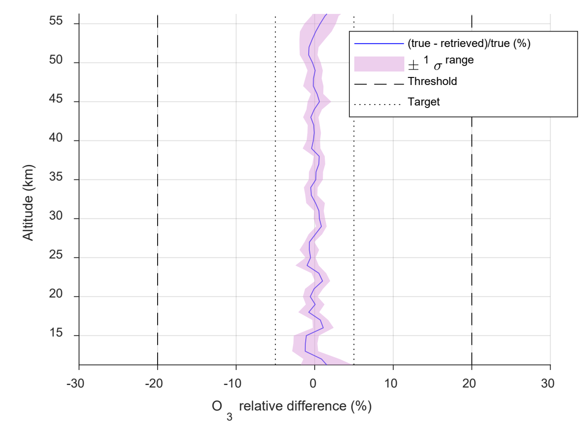
The algorithm follows the maximum a posteriori formalism, with a Levenberg-Marquardt optimization for the iterations.

Like in the bright limb chain, **the number of unknowns is reduced by using a PCA-based representation of the O_3 profile**.

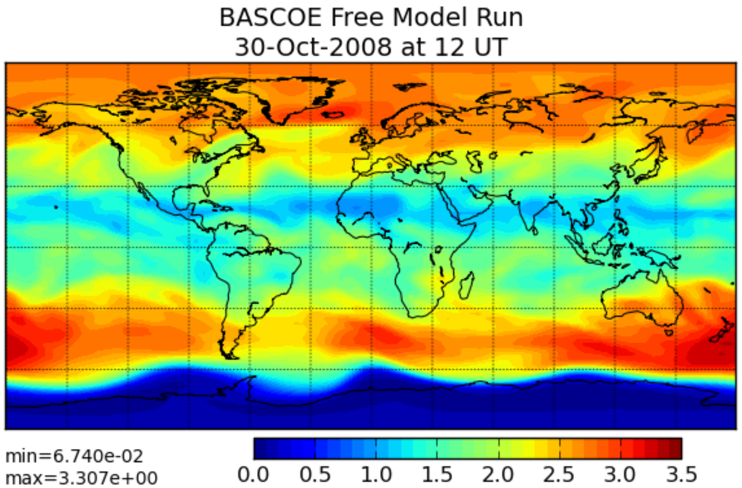


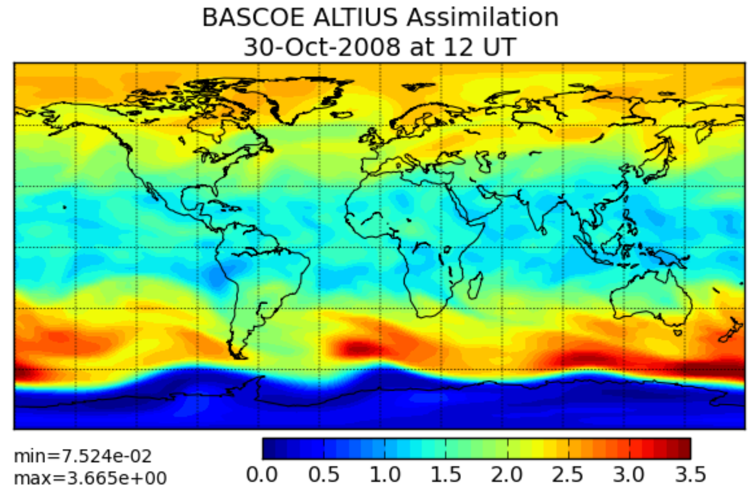


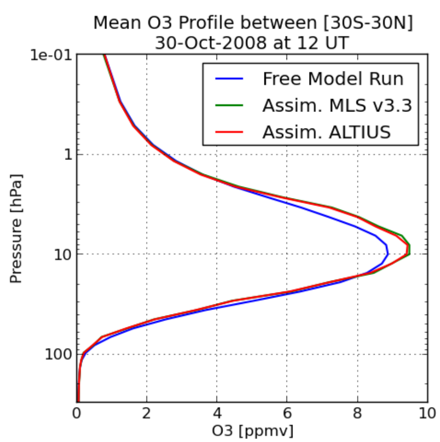


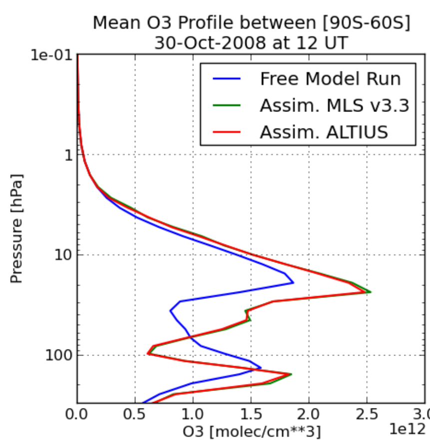


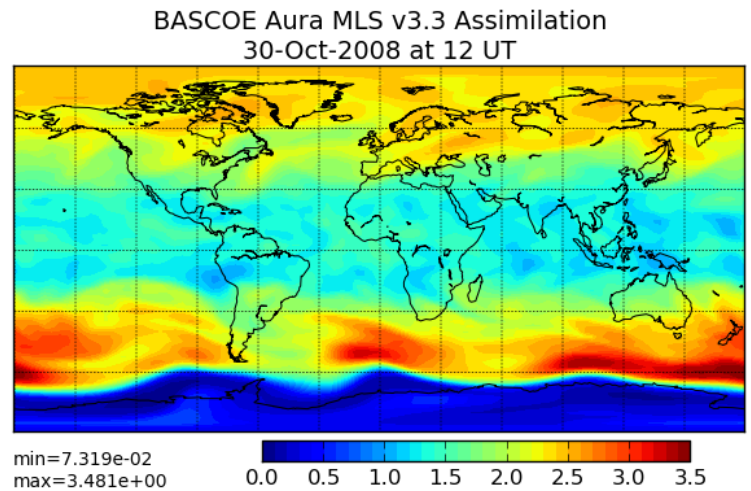
ALTIUS and Aura MLS assimilations are comparable











See f.i. "On the capability of the future ALTIUS ultraviolet–visible–near-infrared limb sounder to constrain modelled stratospheric ozone" Errera et al., Atmos. Meas. Tech., 14, 4737–4753, 2021

ALTIUS ozone retrieval: summary

BRIGHT LIMB

- The description of an ozone profile by an expansion in orthogonal functions (PCA) allows for a clear definition of the number of degrees of freedom and therefore for a clear application of the reduced chi-squared statistics.
- The use of a LUT-NN for radiative transfer leads to a very fast forward model and easy numerical differentiation. Two loops in NRT. The merit function minimization (loop1) is also very fast and can be repeated (loop2) once the resolution is increased till satisfactory chi-squared is achieved.
- SUITLA 2.0 does NOT use
  - any regularization to achieve profile smoothness
  - any optimal estimation method wrt a priori covariance
- Instead, the retrieval algorithm adapts the vertical resolution to the available signal SNR.
- The algorithm is robust. Many potential improvements are open: number of wavelengths/multiplets, finer chi-squared threshold, normalization altitudes,..etc

OCCULTATION

- ALTIUS will observe solar, stellar, planetary, and lunar occultations, ideally extending the geographical coverage and allowing nighttime atmospheric composition sensing
- The O_3 retrieval algorithm has been tested on GOMOS L1 data
- Based on the processing of a set of GOMOS occultations, the scintillation mitigation approach delivers encouraging results.
- Improvement of the regularization scheme, and the retrieval of other species is the next step.