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Ozone_cci round-robin methodology for nadir ozone profile validation using ozonesonde and lidar network data

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Acknowledgements: ESA Ozone_cci, BelSPO/ProDEx A3C and NDACC

NORS/NDACC/GAW Workshop, Brussels, Belgium, 5-7 Nov. 2014

Challenges of nadir ozone profile validation for climate users

1. Several Quality Indicators needed by users cannot be accessed by classical ground-based comparisons.
2. Nadir profile validation is a complex task due to large vertical smoothing errors, high variability etc.

→ Establishment of unbroken QA/validation chain addressing user requirements, in support to ESA's Ozone_cci round-robin selection of nadir algorithms
[Keppens et al., AMTD, 2014]

Table 7: Product requirements for nadir-based ozone profiles. The tropospheric altitude domain extends from the surface to the tropopause defined by an ozone concentration of 150 ppbv; the UT/LS extends from about 5 to 25 km, and the middle atmosphere extends from about 25 to 60 km altitude. The required coverage is global. Achievable and future target requirements are given, separated by a '–'.

Quantity	Driving Research topic	Height range		
		Troposphere	UT/LS	Middle Atmosphere
Horizontal resolution	Regional differences in evolution of the ozone layer and tropospheric ozone burden (radiative forcing); Seasonal cycle and interannual variability; Short-term variability*	20 – 200 km	20 – 200 km	20 – 200 km
Vertical resolution	Height dependence of evolution of the ozone layer and the tropospheric ozone burden (radiati… forcing); Seaso… and inte…	6 km – Tropo…		3 – 10 km
Observation frequency	…ozone la… …e tropospheric ozone burden (radiative forcing); Seasonal cycle and interannual variability; Short-term variability*	3 days	3 days	3 days
Time period	Evolution of the ozone layer and tropospheric ozone burden (radiative forcing)	(1980-2010) – (1996-2010)	(1980-2010) – (1996-2010)	(1980-2010) – (1996-2010)
Accuracy	Evolution of the ozone layer and tropospheric ozone burden (radiative forcing)	10 %	8 %	8 %
Accuracy	Seasonal cycle and interannual variability; Short-term variability*	20 %	15 %	15 %
Stability	Evolution of the ozone layer and tropospheric ozone burden (radiative forcing); trends	1 – 3 % / decade	1 – 3 % / decade	1 – 3 % / decade

[Ozone_cci_URD_2.1, 2011]

Ozone_cci round-robin evaluation

ESA Climate Change Initiative – ECV ozone

Phase-I (2010-2013): Round-robin exercise to verify compliance with climate user requirements (including GCOS) and to identify best parts of 2 different nadir ozone profile retrieval algorithms:

- OPERA v1.26 (KNMI)
- RAL v2.1 (RAL)

applied to measurements from:

- ERS-2 GOME (1997)
- MetOp-A GOME-2 (2007-2008) → see examples

Phase-II (2014-2016): Full reprocessing and validation of GOME, GOME-2A, SCIAMACHY, and OMI with selected algorithm

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QA/Validation Chain

Recommended QA/Validation methodology:

0. Translation of user requirements into validation requirements

THIS TALK

1. Satellite data selection, filtering and post-processing
2. Data content study (DCS) of satellite dataset
3. Information content study (ICS) of satellite dataset
4. Selection and characterisation of correlative data
5. Identification and characterisation of co-located data pairs
6. Homogenization: Resampling, smoothing, and conversions of representation systems and units
7. Data comparisons: bias, spread, stability, dependences…

8. Derivation of Quality Indicators
9. Discussion of compliance with user requirements

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QA/Validation

Recommended QA/Validat

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2. Data content study (D
3. Information content st
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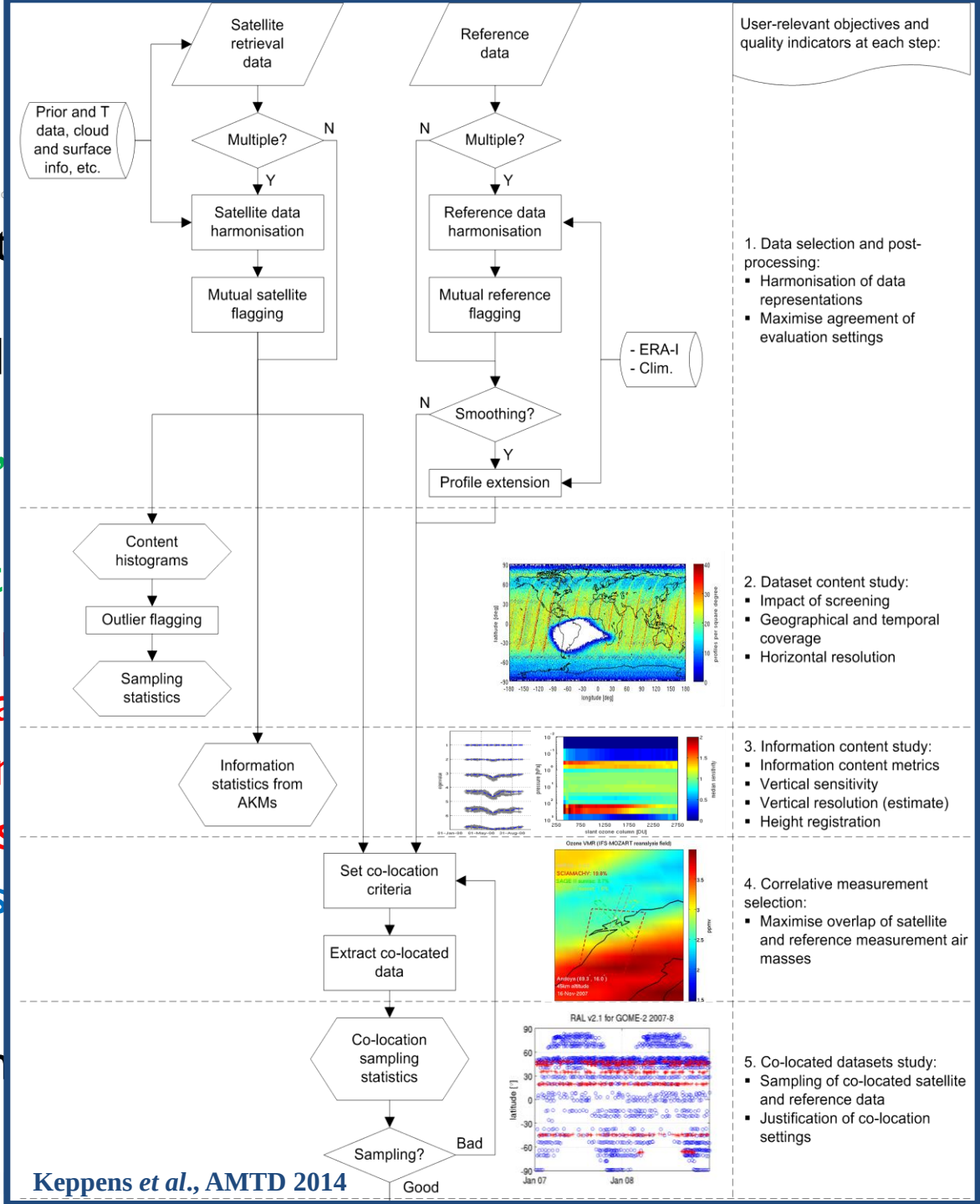
5. Identification and chara
6. Homogenization: Resar representation systems
7. Data comparisons: bias

8. Derivation of Quality I
9. Discussion of complian



Keppens *et al.*, AMTD 2014

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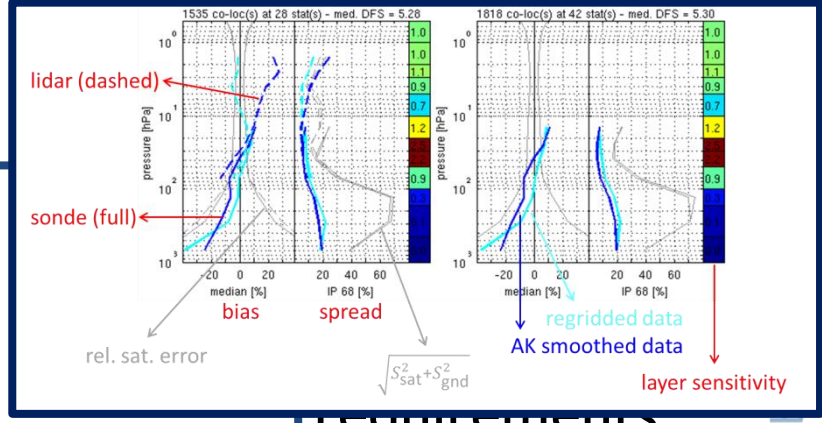
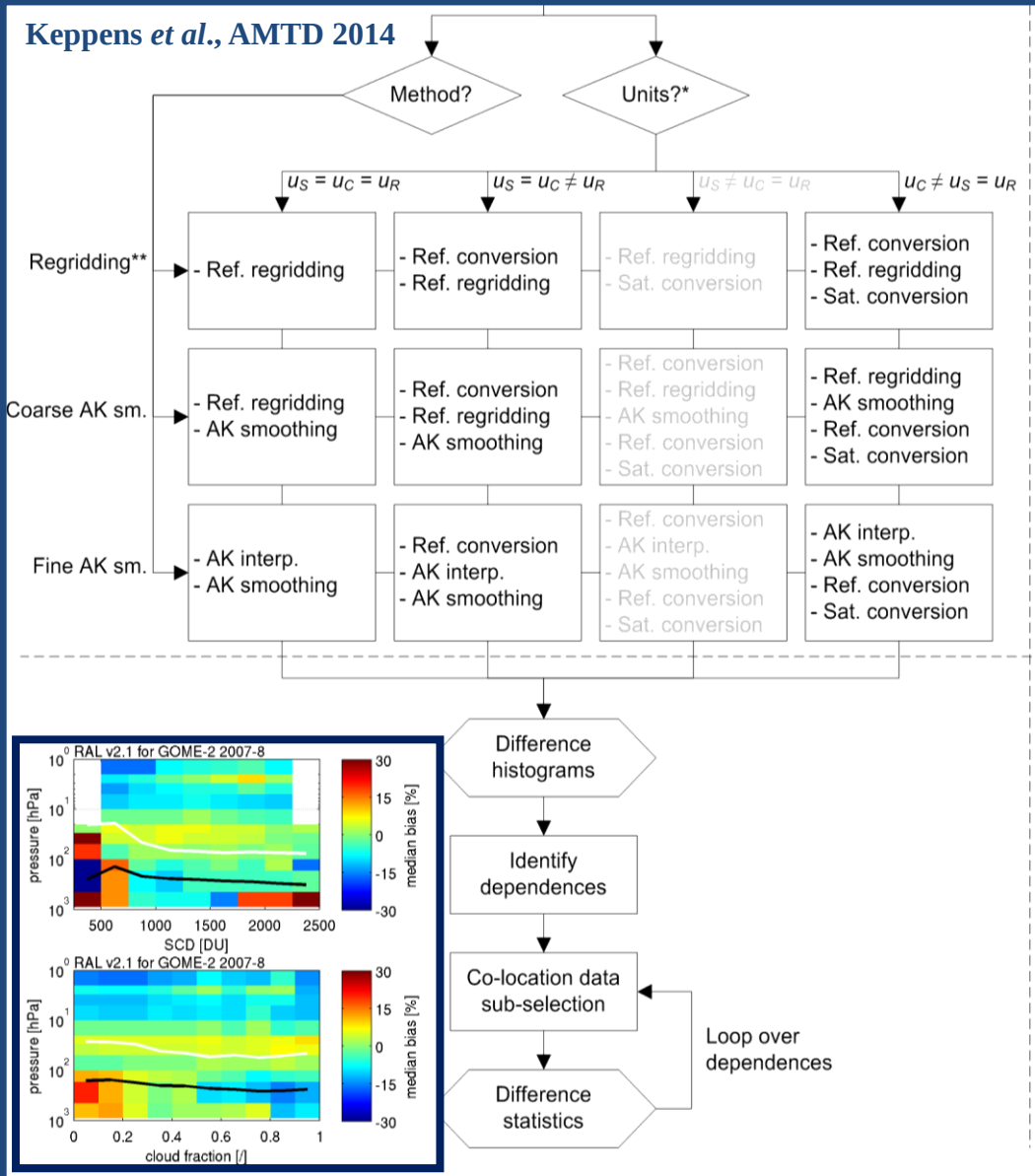
OA/Validation Chain



Keppens *et al.*, AMTD 2014



6. Vertical resampling of reference profiles:
   - Common vertical grid
   - Apply satellite measurement smoothing to reference profile

7. Comparisons:
   - Difference average (bias) as measure for satellite accuracy
   - Total satellite uncertainty estimation by combining bias and random satellite uncertainty or bias and comparison spread
   - Comparison bias and spread dependences on physical conditions and/or retrieval metadata
   - Difference timeseries for stability analysis

* u_S, u_C, and u_R for satellite, comparison, and reference units, respectively.
** Regridding only, or regridding including function smoothing (Gaussian, triangular, others). Regridding possibly by summation for sub-columns.

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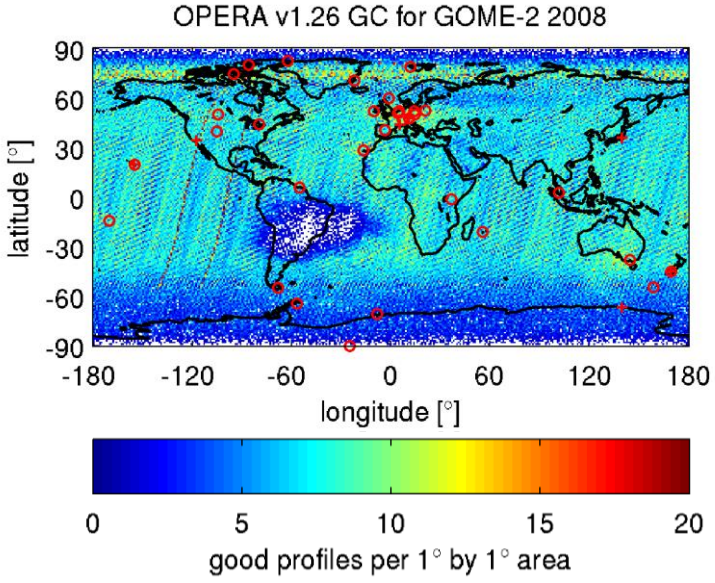
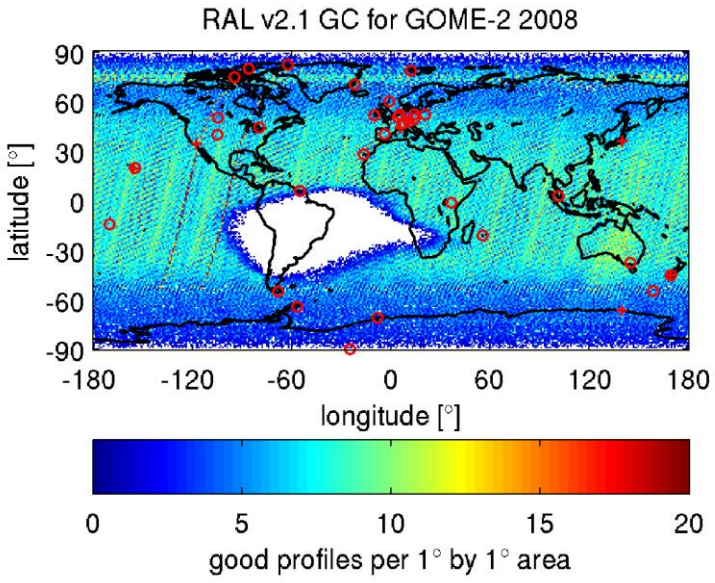
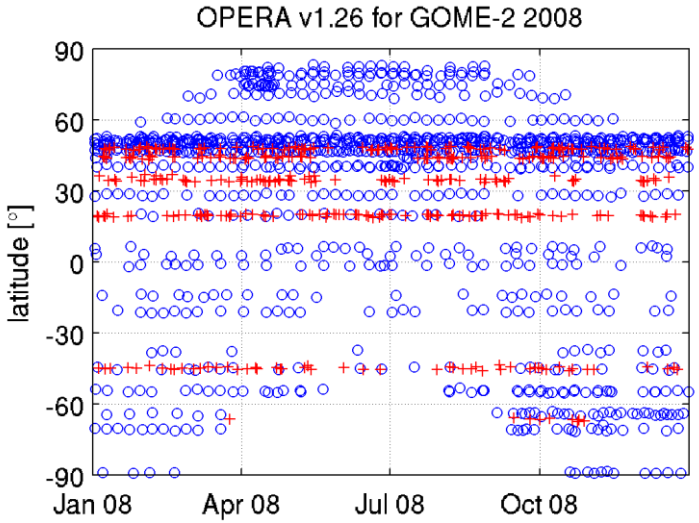
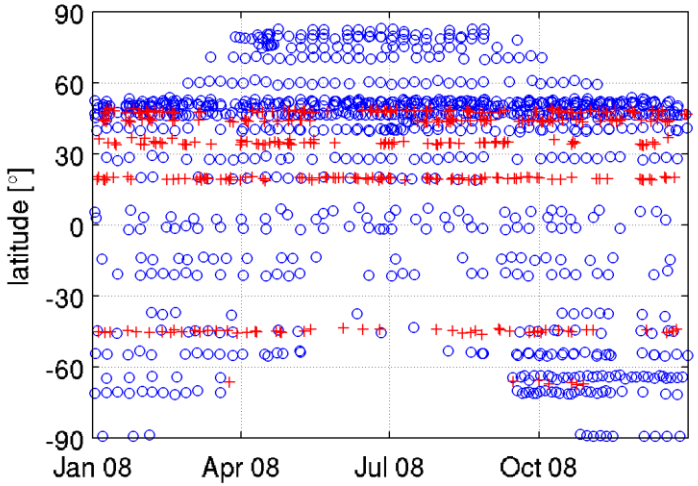
Data content and co-location studies

Example: Spatio-temporal sampling









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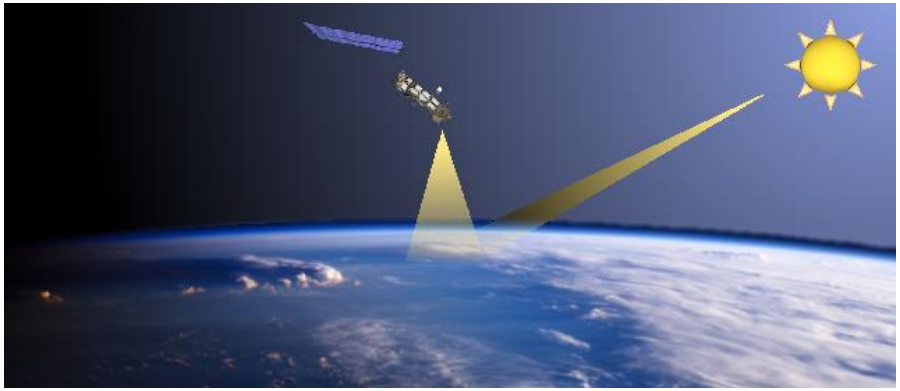
Information content study

- Characterize the sensitivity of the measurement to the actual state of the atmosphere, in terms of independent information (DFS), vertical resolution, and uncertainty in height registration.
- Estimated from the Averaging Kernels (AK), product of Jacobians of inverse model and forward model:

$$\bar{x} = x_a + A(x - x_a) + \varepsilon_x$$

- AKs depend on SZA, SCD, clouds, etc.
- Fractional kernels required for unit-independent analysis!



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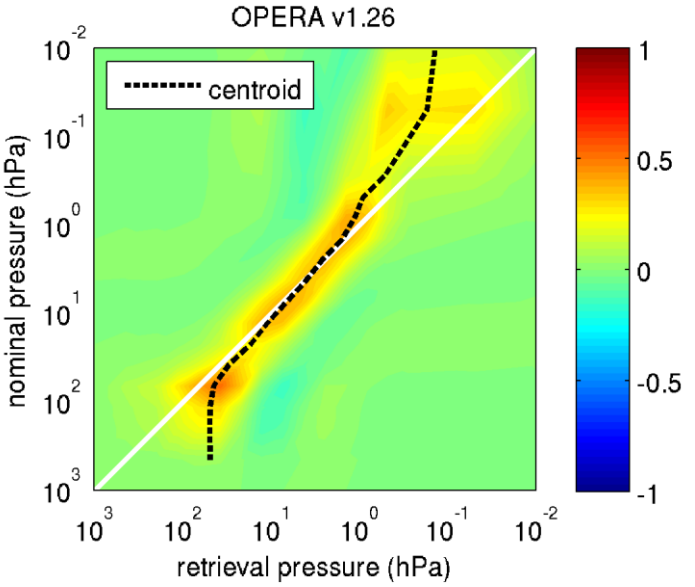
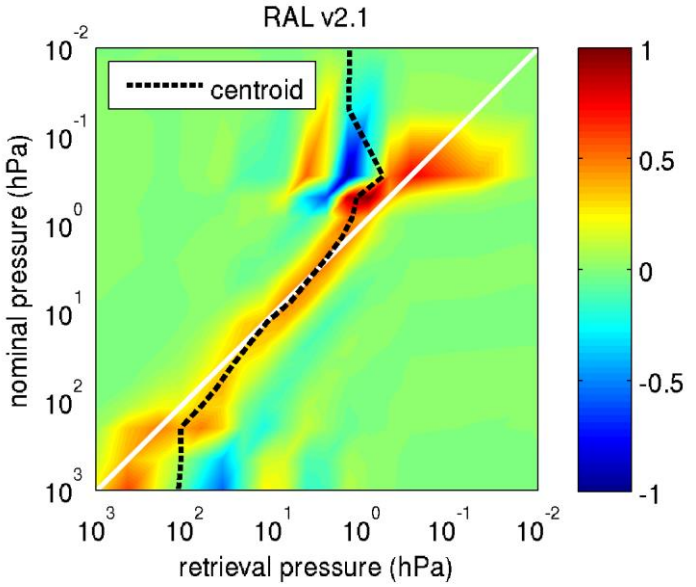
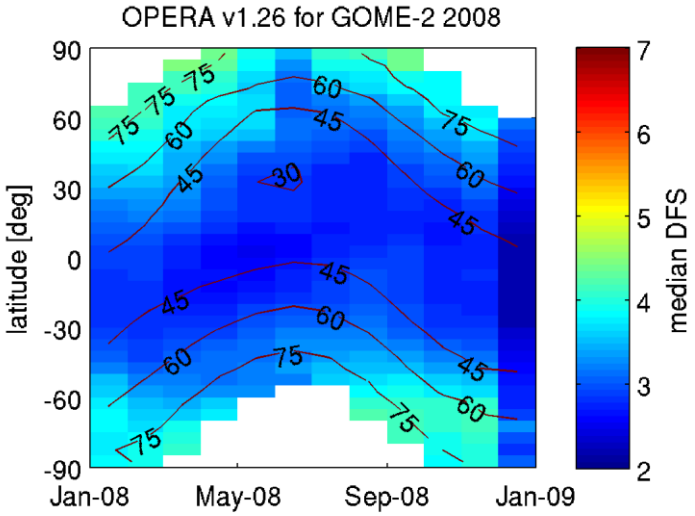
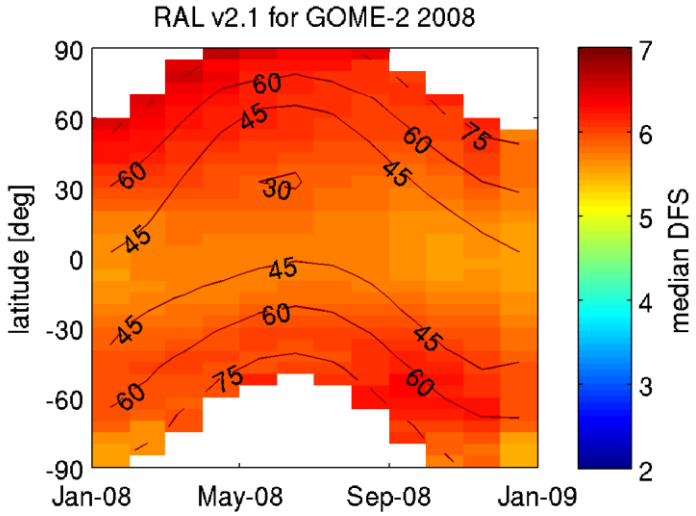
Information content study

Example: Height registration/resolution and DFS









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Data homogenization

Smoothing using column conservation [Calisesi et al., JGR, 2005]
→ Reference data remain independent from the data being validated

Smoothing using AKs: $\bar{x}_g = A \times \bar{x}_g + (I - A) \times x_p$
→ Requires regridding of the high-resolution reference data

Smoothing using interpolated AKs: $\bar{x}_g = A^* \times x_g + (I - A) \times x_p$
→ Requires interpolation of AKM rows

Smoothing using interpolated AKs: $\bar{x}_g = x_p + A^* \times (x_g - x_p^*)$
→ Requires interpolation of AKM rows AND prior profile

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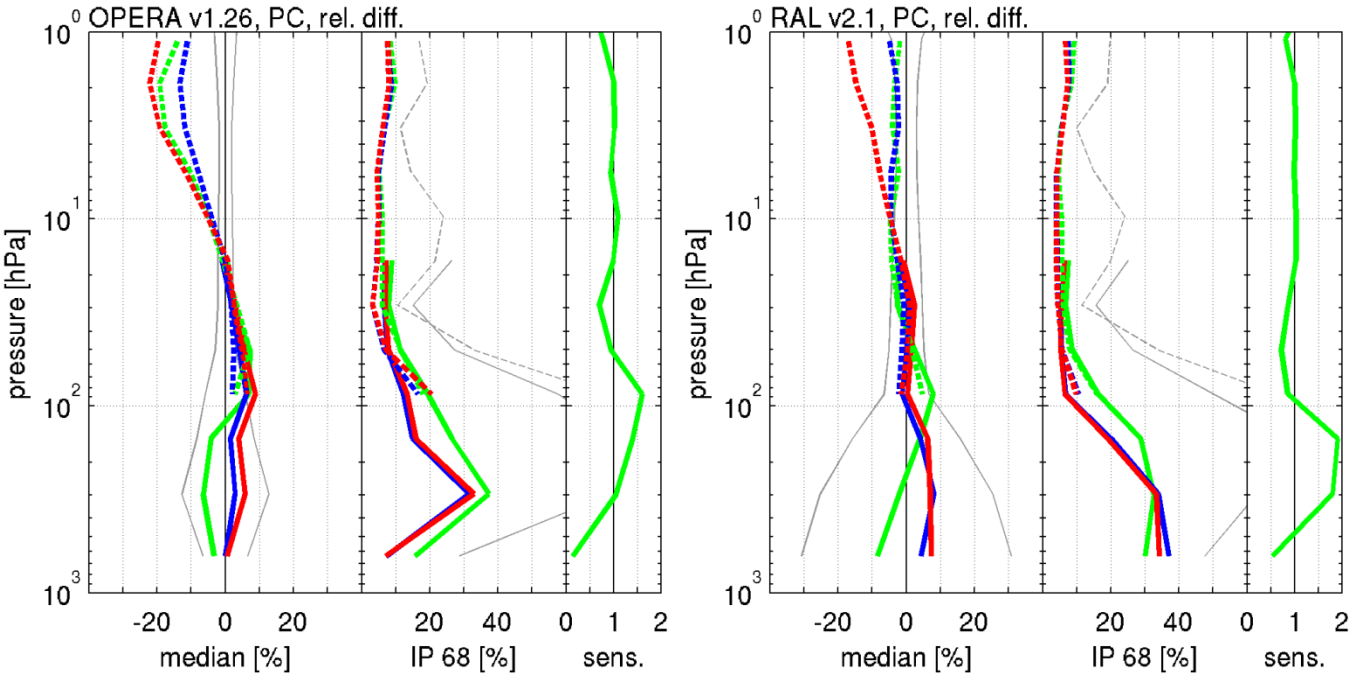
Data comparison

Example: Bias & spread

- vs. GAW/NDACC/SHADOZ ozonesondes & NDACC lidars
- Vertical sensitivity & Calisesi smoothing (green)
- AK smoothing: coarse AK (blue) vs. fine resolution AK (red)
- Unit conversion: PC (left) vs. PC from ND (right)



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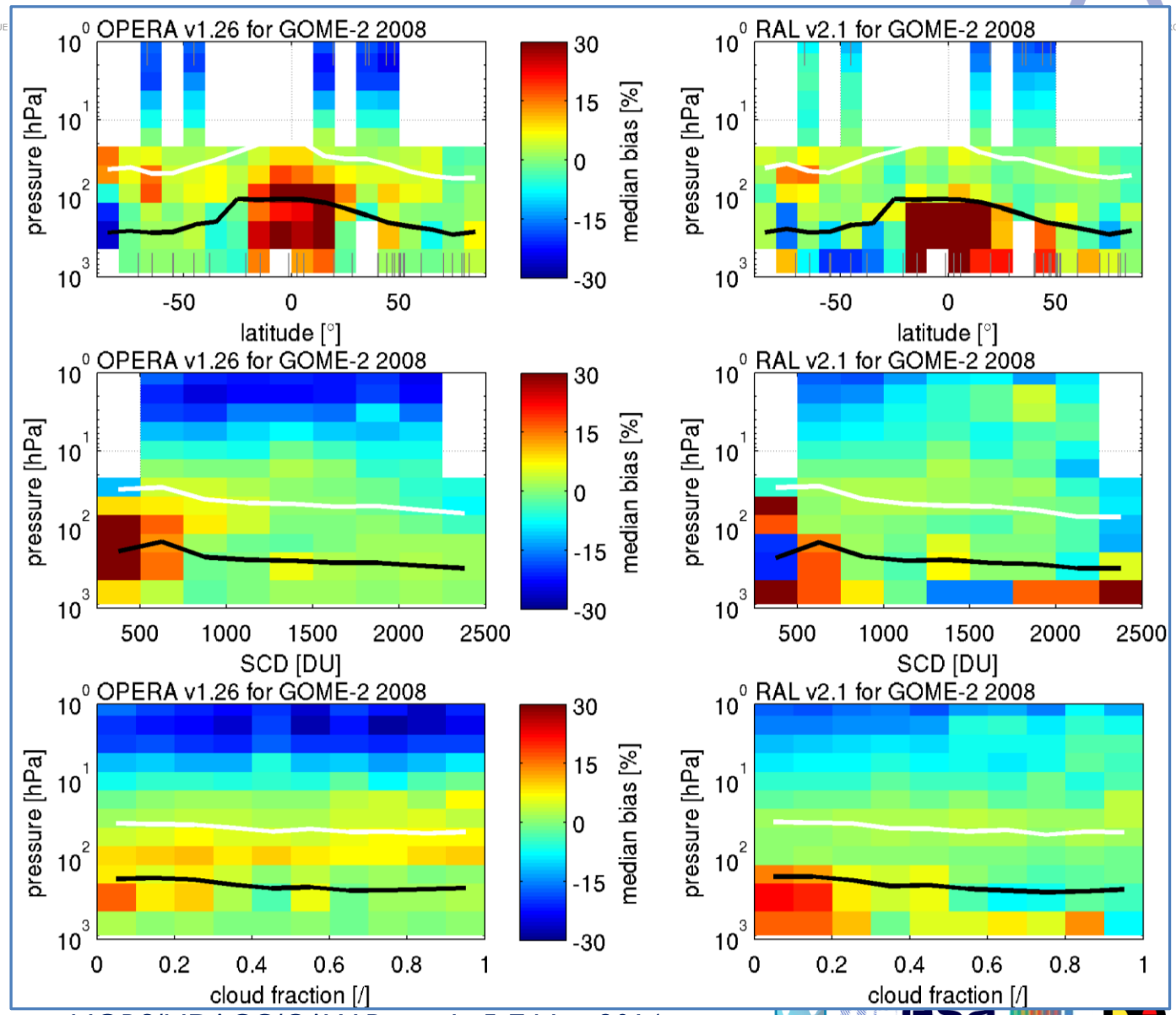
Data comparison

Example: Dependences

- Time
- Latitude
- Slant column
- Cloud fraction

Ozone peak (white)

WMO tropopause (black)



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Compliance with user requirements

Example: CCI round-robin summary table

NADIR L2	Part atmos.	URD / PVP	OPERA v1.26 GOME-2 (2008)	RAL v2.1 GOME-2 (2008)
Filtering			~10%	~ 10 %
Geo. sampling			Full	SAA missing
DFS			3 to 4	5 to 6
Vertical resolution (resolving length estimate)	TS	6 km to TS-col.	> 40 km	> 40 km
	UT/LS	3 to 6 km	10 to 20 km	10 to 20 km
	MA	3 to 10 km	20 to 40 km	> 40 km
Height registration offset	TS	/	10 to 20 km	10 to 15 km (SZA dep.)
	UT/LS		negligible	negligible
	MA		-20 to 0 km	-20 to 0 km
Accuracy (bias)	TS	/	~ 5% (1 DU)	7 to 8 % (1 DU)
	UT/LS		-5 to 10% (-1 DU to 3 DU)	1 to 4 % (1 DU)
	MA		-20 to -5% (-2 DU to -1 DU)	-15 to 0 % (-3 to 0 DU)
Temporal dep.		/	NH summer: positive bias between TP and O3 max.	Increased bias around and below TP for NH winter
Meridian dep.	60-90	/	Neg. around SP TP; Pos. around SP O3 max.	Neg. bias around and below TP, positive around ozone max.
	30-60		Small pos. biases	Neg. bias below TP
	0-30		Pos. bias up to O3 max	Increased bias below TP, related to bias for small SCD values
SCD dep.			Clearly related to meridian dependence	Clearly related to meridian dependence
CF dep.			Positive around TP when cloud free	Slightly decreasing (more negative) bias with CF
Comparison spread	TS	/	10 to 30% (1 to 4 DU)	30 to 35 % (4 to 5 DU)
	UT/LS		~5% (3 DU)	5 % (3 DU)
	MA		5 to 10% (0 to 3 DU)	5 to 10 % (0 to 3 DU)
Satellite random uncertainty	TS	/	6 to 12%	10 to 30 %
	UT/LS		2 to 5%	~5%
	MA		2 to 3%	3 to 5 %
Total uncertainty	TS	10%	8 to 30%	12 to 36 %
	UT/LS	8%	5 to 11%	5 to 7 %
	MA	8%	5 to 22%	3 to 18 %

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Summary

An unbroken QA/validation chain for nadir ozone profile retrievals has been formulated, which provides the set of quality indicators enabling climate research data users to fully assess the fitness-for-purpose of nadir ozone profile data.

This "best practice" includes a suite of data manipulations and dataset studies yielding complementary perspectives on data quality:

- Detailed data and information content studies
- Careful treatment of representation, sampling and smoothing issues
- Comparisons with respect to ground-based reference measurements and multivariate statistical analysis

as illustrated on two MetOp-A GOME-2 retrievals.

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