wege entstehen, indem wir sie gehen
paths emerge in that we walk them

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Reference Occultation Processing System (rOPS) for cal/val and climate: a new GNSS RO retrieval chain with integrated uncertainty propagation

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Thanks to all further colleagues at WEGC (ARSCliSys Research Group) and all partners worldwide for valuable discussions and advice! See next slide for international advisers and cooperation partners…

Thanks for funds to esa, asap FFG, FWF

IROWG-4 International Workshop, Bureau of Meteorology, Melbourne, Australia, 16-22 April 2015

rOPS international advisers and cooperation partners

- EUMETSAT: Axel von Engeln, Christian Marquardt, Riccardo Notarpietro, Yago Andres, Yoke Yoon
- DMI, ECMWF: Stig Syndergaard, Kent Lauritsen, Sean Healy
- UCAR, JPL: Bill Schreiner, Doug Hunt, Tony Mannucci, Chi Ao
- IAP, TUG: Michael Gorbunov, Torsten Mayer-Gürr
- AIUB, DLR: Adrian Jäggi, Oliver Montenbruck
- NSSC/CAS, IGG/CAS, RMIT: Congliang Liu, Ying Li, Kefei Zhang

…and more may join as the work proceeds…thanks all!

Two main lines of cooperation:

- joint papers (on specific rOPS-related key issues to be solved)
- advice & expert meetings (~1-day review/advice meetings at WEGC)

motivation 1: why rOPS? – three views, one goal

Address WEGC's overarching research question#1 (from its research strategy 2013-2017), for thermodynamic ECVs:

- How can we solve the global climate monitoring problem in the atmosphere? That is, how can we provide authoritative benchmark climate records of essential climate variables (ECVs) such as temperature, humidity, wind, and greenhouse gases like CO_2 and CH_4? => rOPS: solve it for (φ, *d*, α, *N*,) ρ, ***p***, *Z*, ***T***, (partially) ***q***.

Address Rick Anthes' claim that he (again) emphasized in his opening talk at OPAC-IROWG 2013 and IROWG-4 2015:

- "GNSS radio occultation is the most accurate, precise, and stable thermometer from space." => rOPS: prove it for atmospheric *T*.

Address a decades-long demand by IPCC, WCRP, WMO/GCOS,…:

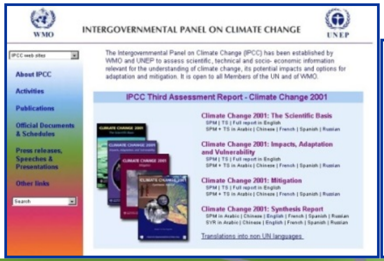
- Accurate, long-term, consistent data, traceable to SI standards and providing a benchmark, are the backbone of contemporary climate science. => rOPS: provide it for atmospheric thermodyn ECVs.

We must monitor the atmosphere and climate with benchmark data techniques since…

…these unique data serve as fundamental backbone and "true" reference standard to atmosphere and climate science & services,

and more specifically, three major reasons:

- to rigorously observe and learn, independent of models, how weather and climate variability and change evolve, over monthly, seasonal, interannual, and decadal scales
- to test and guide the improvement of weather and climate models and thereby enhance their predictive skills for estimating future weather and climate
- to use the data as accurate observational constraints for natural and anthropogenic climate change detection and attribution



*...from the 9 **"high priority areas for action"** noted in the **IPCC 2001 report** (Summary for Policymakers, IPCC WG I, p. 17) - **still valid 14 years later in 2015:***

*"- **sustain and expand the observational foundation for climate studies by providing accurate, long-term, consistent data including implementation of a strategy for integrated global observations.**"*

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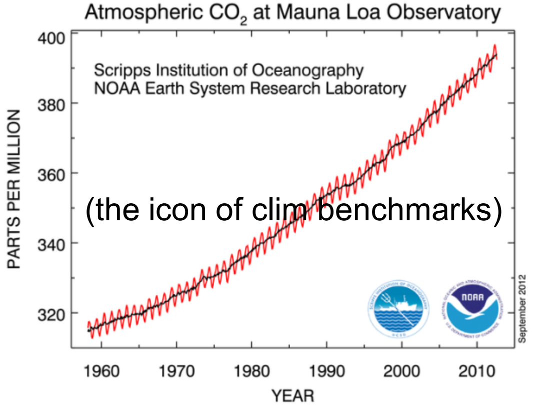
Which properties need such benchmark data to have and can GNSS RO provide these?

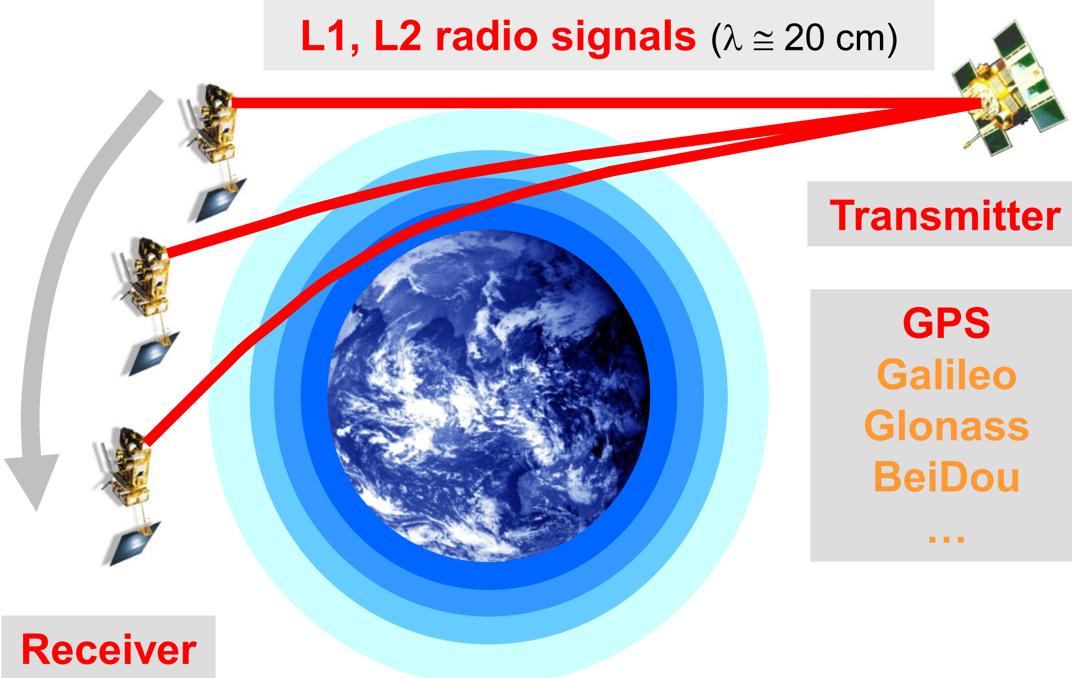
Key properties:



- long-term stable (over decades and longer)
- accurate (traceable to SI standards)
- globally available (same above land and oceans, etc.)
- measure sensitive indicators of atmosphere and climate change, in a physically consistent manner, in particular: => GCOS Essential Climate Variables (ECVs) (in the atmosphere: temperature, pressure, water vapor, wind, greenhouse gases, etc.) [e.g., GCOS Guideline, GCOS-143(WMO/TD No. 1530), May 2010]

GNSS RO can provide such data for thermodynamic core ECVs over the (free) troposphere and stratosphere.

GNSS RO – the principle and the promise



(basic fig courtesy U. Foelsche WEGC)

Satellites in Low Earth Orbit:

GPS/Met (1995-97), CHAMP (2001-08), SAC-C, GRACE, F3/COSMIC, MetOp-A & -B, TerraSAR-X,…

- setting & rising RO events in an active limb sounding mode exploit the
- atmospheric refraction of (two) GNSS L-band signals, providing
- *self-calibrated measurements* of atm. excess phase path / Doppler shift *traceable to fundamental time* (SI second) for the retrieval of
- bending angle α and in turn key atm&clim variables (core ECVs) refractivity, density N, ρ, pressure, geopot.height p, Z, temperature T, humidity q

*The **RO promise** for climate (and beyond) – unique combination of:*

+ high accuracy & long-term stability (from SI traceability), at high vertical resolution; regular, all-weather global coverage;

=>bench-qual reference processing needed to really meet the promise=>rOPS.

RO processing – existing schemes have limited potential to serve as reference processing system…

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Processing Center	Data version	Processing Steps [a]
DMI Copenhagen, DK	OCC_20.6.688, FM_2.1 (UCAR/CDAAC 2009.2650)	UCAR phase & orbit data Geometrics optics (GO), CanonTransf (CT)<25 km Optimization of *α* with MSISE-90 (>40 km)
EUM Darmstadt, D	YAROS 0.1(Beta) – ROTrend_5.1_Prof (UCAR/CDAAC 2009.2650)	UCAR phase & orbit data GO Optimization of *α* with CIRA-MSISE
GFZ Potsdam, D	POCS ATM vers.006	Excess phase single differencing GO, Full Spectrum Inversion (FSI) <15 km Optimization with MSISE-90 (>40 km)
JPL Pasadena, CA, USA	v2fo_10Kp1N	Excess phase double differencing CT Exponential function fit of *α* at 40–50 km, extrapol.
UCAR Boulder, CO, USA	2009.2650	Excess phase single differencing GO, Full Spectrum Inversion in troposphere Optimization with NCAR climatology
WEGC Graz, A [Summary after Steiner et al. *ACP* 2013]	OPSv5.4 (UCAR/CDAAC 2009.2650)	UCAR phase & orbit data GO Statistical optimization >30 km with ECMWF forecasts & MSISE90 above

[a] All centers: ionospheric correction of bending angles and dry air retrieval but different smoothing routines and different quality control; for details, including Tables on the schemes, see Ho et al. *JGR* 2012 and Steiner et al. *ACP* 2013 (known to the experts here)

existing schemes – status is good in core region but… (1)

Atmos. Chem. Phys., 13, 1469–1484, 2013
www.atmos-chem-phys.net/13/1469/2013/
doi:10.5194/acp-13-1469-2013

Atmospheric Chemistry and Physics
Open Access

Quantification of structural uncertainty in climate data records from GPS radio occultation

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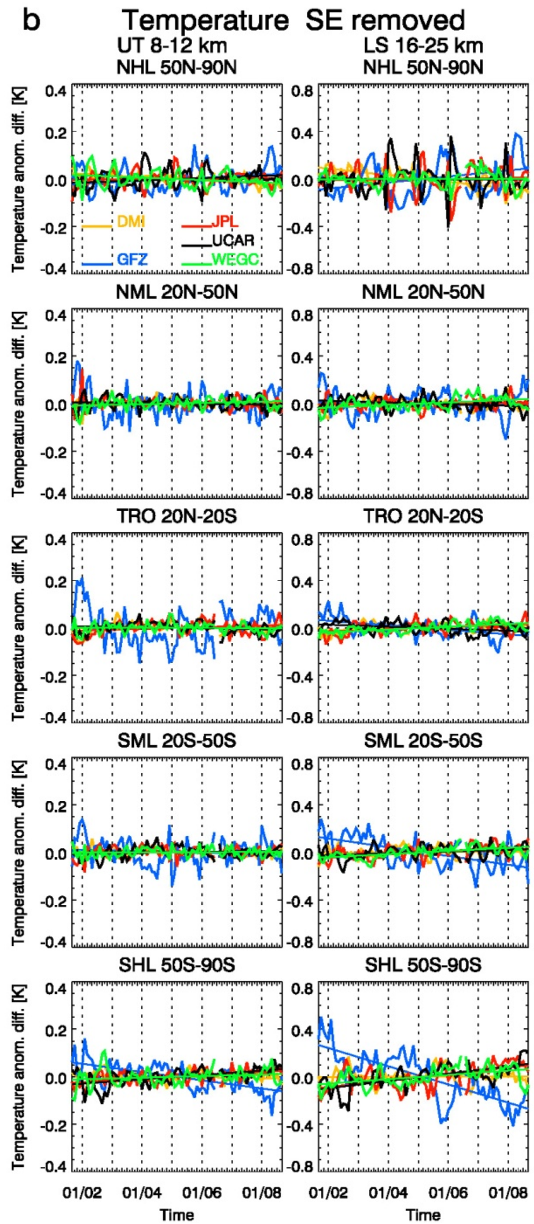

"…Larger structural uncertainty above about 25 km and at high latitudes is attributable to differences in the processing schemes…climate trend assessment is bound to 50°S to 50°N…" *=> We need more…*

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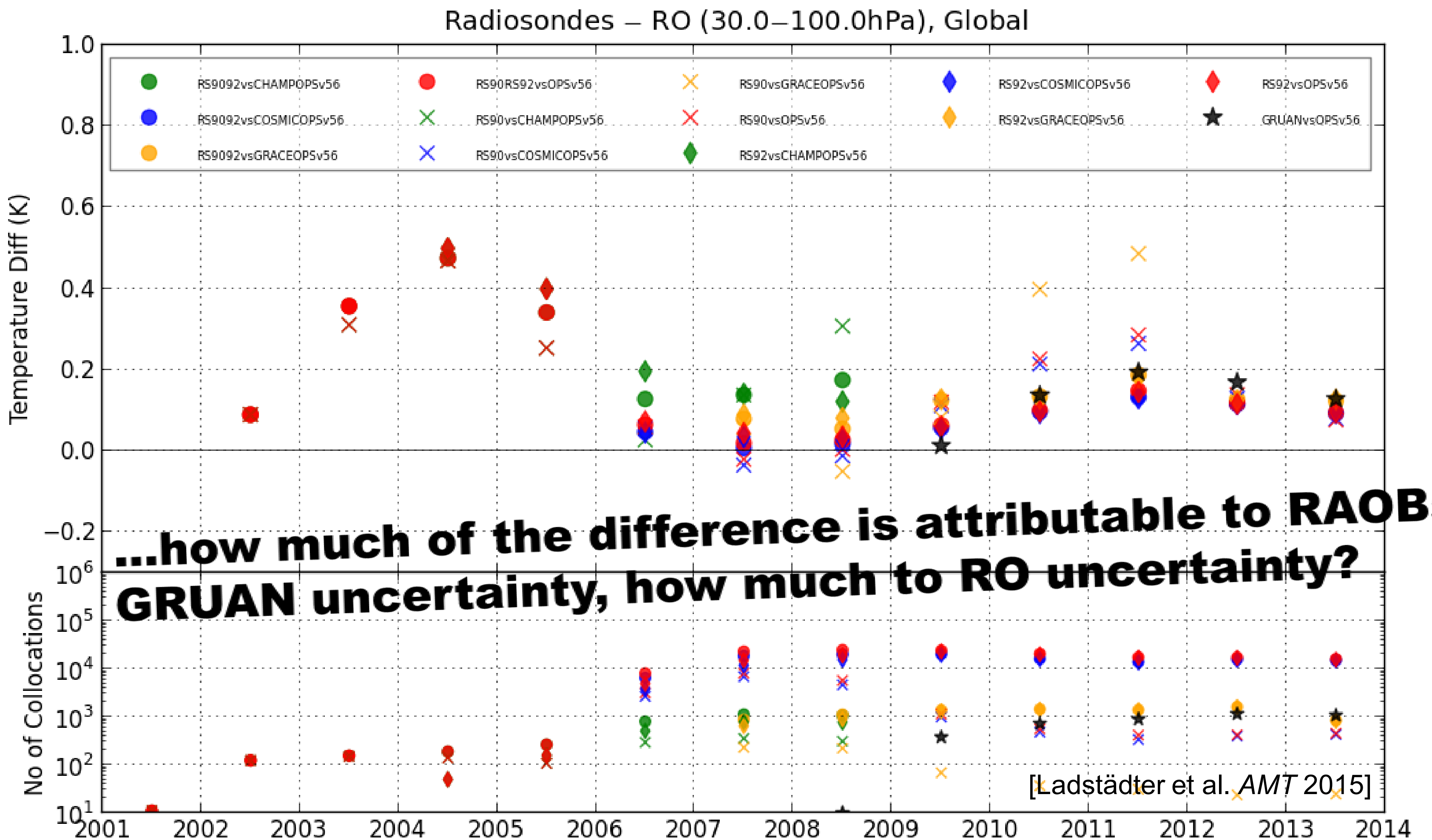
RAOBs V90/92 and GRUAN vs RO-OPSv5.6 CHAMP, GRACE, COSMIC

- Annual-mean temp differences (global, example altitude range 100hPa–30hPa)

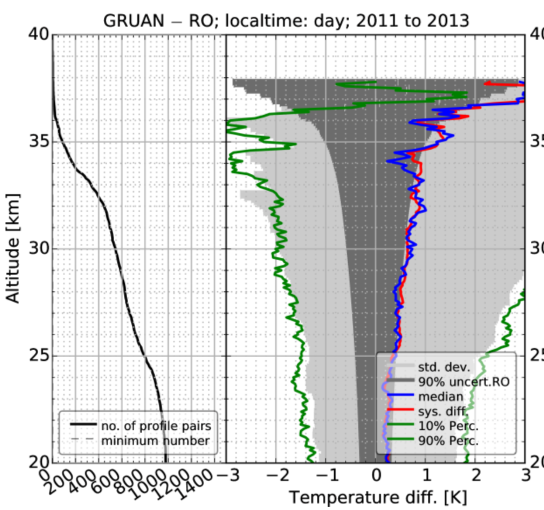


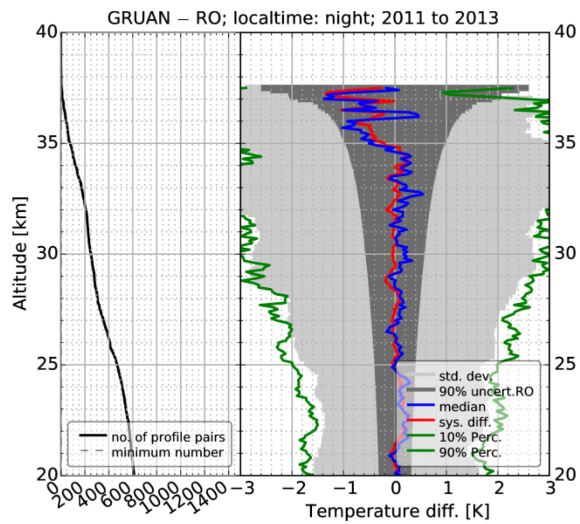
…how much of the difference is attributable to RAOBs & GRUAN uncertainty, how much to RO uncertainty?

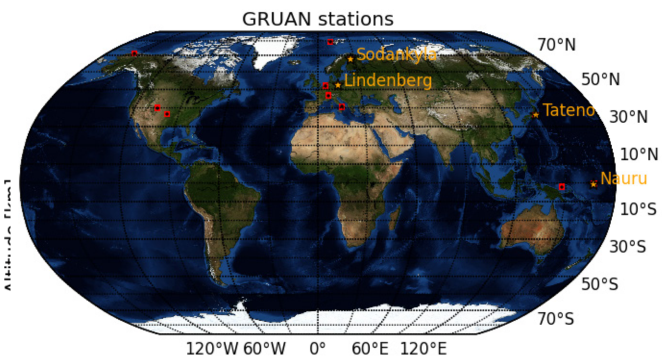
[Ladstädter et al. *AMT* 2015]

GRUAN day vs night – use of RO-OPSv5.6 for checking radiation bias

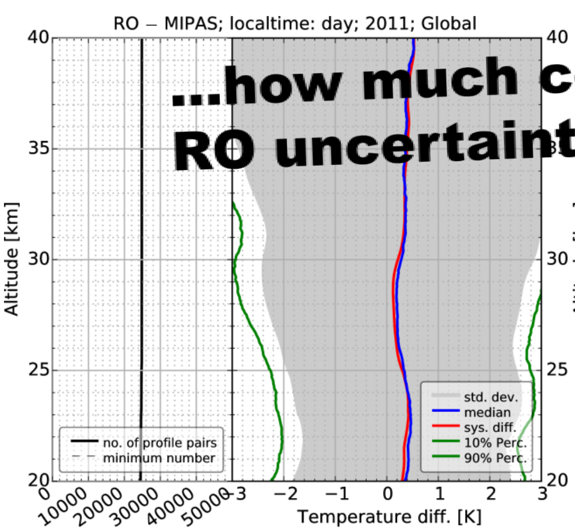
- RO is capable to reveal GRUAN rad bias (as indicated by side-comp to MIPAS)

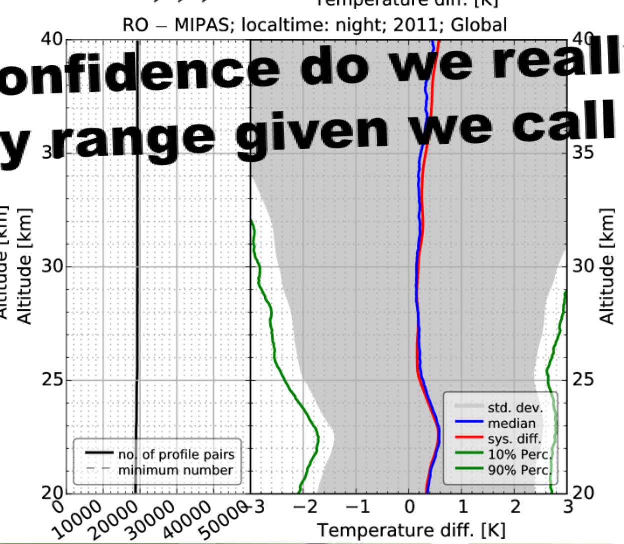






GRUAN vs RO
day (left) & night (right)





…how much confidence do we really have in the current RO uncertainty range given we call MIPAS to our aid?

RO vs MIPAS
day (left) & night (right)

[Ladstädter et al. *EGU-Pres* 2015]

...so again to the RO promise, what‘s next? – rOPS! ☺

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…

[citation from my keynote talk “RO for climate monitoring: where we stand, what’s next…” at Apr.2011 Taiwan COSMIC workshop; from a summary slide]

“ on accuracy & stability:

- ensure high-perform instruments (GRAS-type performance above ~8 km, robust&accurate OL tracking below)
- need new processing systems (compliant to GCOS guidelines and IROWG/climate recommendations; systematic upper stratosphere and troposphere improvements needed; e.g., WEGC OPSv5.4 is end-of-life, to be substituted…by completely fresh “reference OPS”, rOPS)
- document the trace back from excess phase & SNR data to SI standards (reference time, reference power/lower tropo.)”

In fact the rOPS high-level introduction on the next slides indicates its not just quite an improvement over WEGC’s OPSv5.4/OPSv5.6 processing but relative to all existing schemes.

rOPS (1) – goal, processing tracks, processors

Goal: provide bench-qual reference RO data for calibration/validation and for climate monitoring, research, and services, complementary to NRT.

Three processing tracks:

- Fast-track reference (FTR) data: daily on follow-on day of observations
- Postprocess-track reference (PTR) data: daily with three weeks latency
- Re-processing reference (RPR) data: occasionally (kicked of manually), as highest-fidelity climate records over entire multi-satellite periods

Four processors:

- Level 1a processor: Raw data ($L0_p$) to excess phase level data (L1a)
- Level 1b processor: Excess phase/SNR to atmos bending angle (L1b) ($t \rightarrow a$ space; obs only, no bgr info)
- Level 2a processor: Bending angle to refrac and dry-air variables (L2a) ($a \rightarrow z$ space; bgr info from high-altitude initialization only)
- Level 2b processor: Dry-air variables to moist-air variables (L2b) (tropo moist-air retrieval in z space; bgr info on T, q)

One key now, before data processing perform system modeling...

rOPS (2) – systems modeling as basis for data processing

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Two major system layers, each with several subsystems:

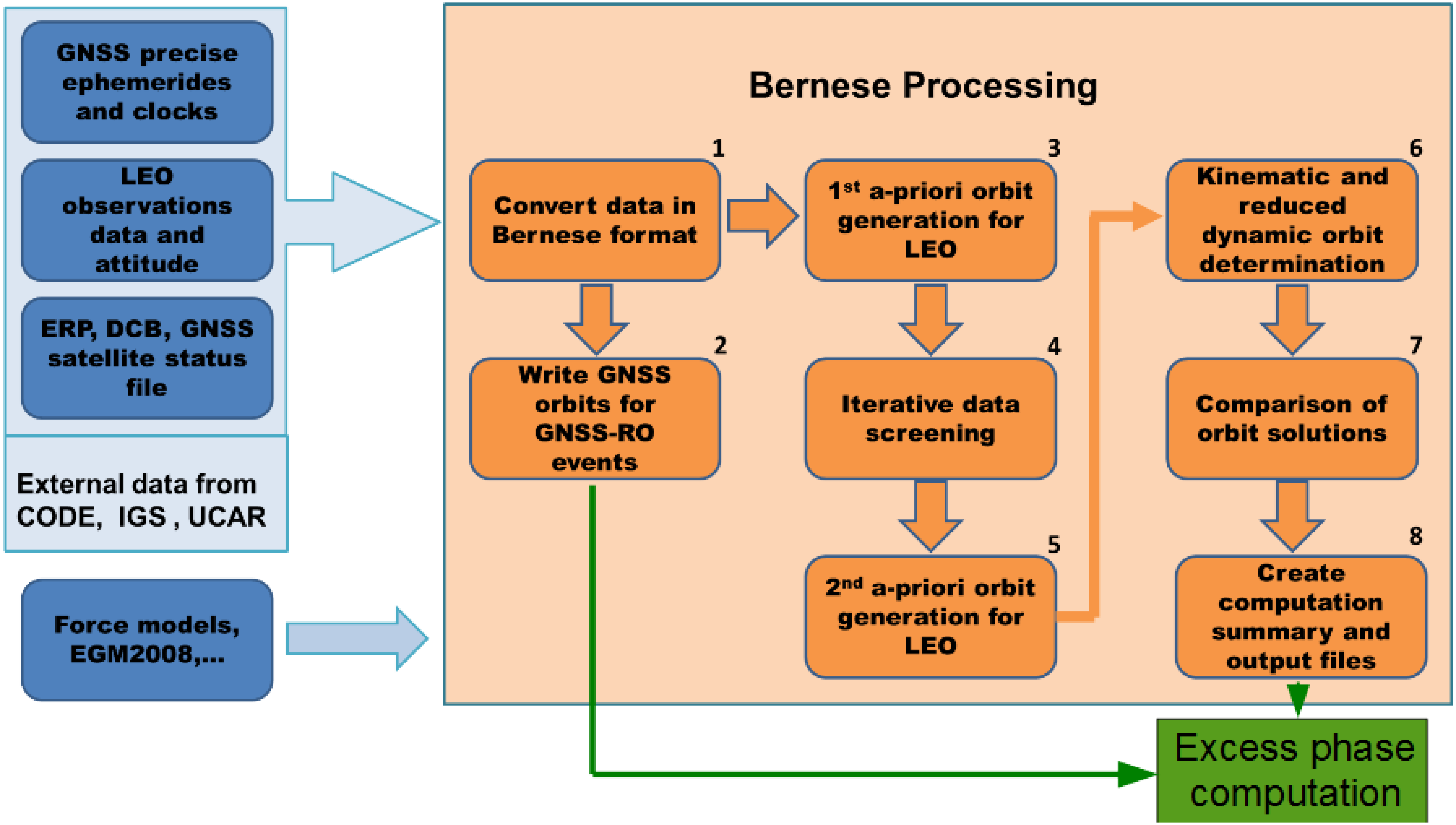
- Background system modeling (daily):
  Atmosphere system (ECMWF An, Fc; OPS Obs-L1b, Obs-L2a)
  Atm.Uncertainties system ($F_{\varphi,\lambda,\tau}(\boldsymbol{x}_a, \boldsymbol{x}_f; \boldsymbol{x}_o)$ weather filters: $\boldsymbol{u}_b$, $\boldsymbol{u}_o$, $\boldsymbol{R}_b$, $\boldsymbol{R}_o$)
  Ionosphere and Ion.Uncert. system (JPL/UCAR IAn $\boldsymbol{x}_{ion}$, $\boldsymbol{u}_{ion}$; NeUoG)
  GNSS Tx system (IGS&CODE $\boldsymbol{x}_G$, $\boldsymbol{v}_G$, τ_G; $\boldsymbol{U}^s_{XG,}$ $\boldsymbol{U}^c_{XG}$)
  LEO Rx system ($\boldsymbol{X}_G$&$\boldsymbol{X}_{L0nav,L}$/Bernese&Napeos $\boldsymbol{x}_L$, $\boldsymbol{v}_L$, τ_L; $\boldsymbol{U}^s_{XL,}$ $\boldsymbol{U}^c_{XL}$)

- Occultation event system modeling (per event):
  RO event geometry model (ECEF/WGS84/EGM96 $\boldsymbol{X}_G$, $\boldsymbol{U}_{XG}$; $\boldsymbol{X}_L$, $\boldsymbol{U}_{XL}$;
  t_{MTP}, $\boldsymbol{x}_{MTP}$, $\boldsymbol{s}_{MTP}$, $R_{C,MTP}$, $\delta\boldsymbol{r}_{C,MTP}$; G_{MTP}, $R_{E,MTP}$)
  RO event L2 data model (ECMWF Fc-L2b, Fc-L2a; JPL/UCAR IAn-L2)
  RO event L1 data model ($F_k(N\rightarrow\alpha\rightarrow d\rightarrow\varphi)$ operators: Fc/IAn-L1b, Fc-L1a)
  RO event vertical grid model ($z \rightarrow z_p$, z_a, $a_z \leftrightarrow a_t$, z_{at}, z_t, $t^s_t \leftarrow t$; $\boldsymbol{X}_{TPT}$)
  RO event geom operators ($\boldsymbol{A}_k$ models for $\varphi\leftrightarrow d\leftrightarrow\alpha\leftrightarrow N\leftrightarrow p_d, T_d\leftrightarrow p, T, q$)

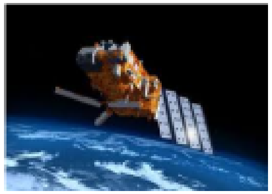
These basic system modeling steps are performed before RO data processing starts (except for $F_{\varphi,\lambda,\tau}(\boldsymbol{x}_o)$ estimates, which precede respective L1b/L2a/L2b procsteps) $\Rightarrow$ informs, assists, and speeds up the processing.

rOPSv1 LEO Rx system modeling – LEO POD processing strategy

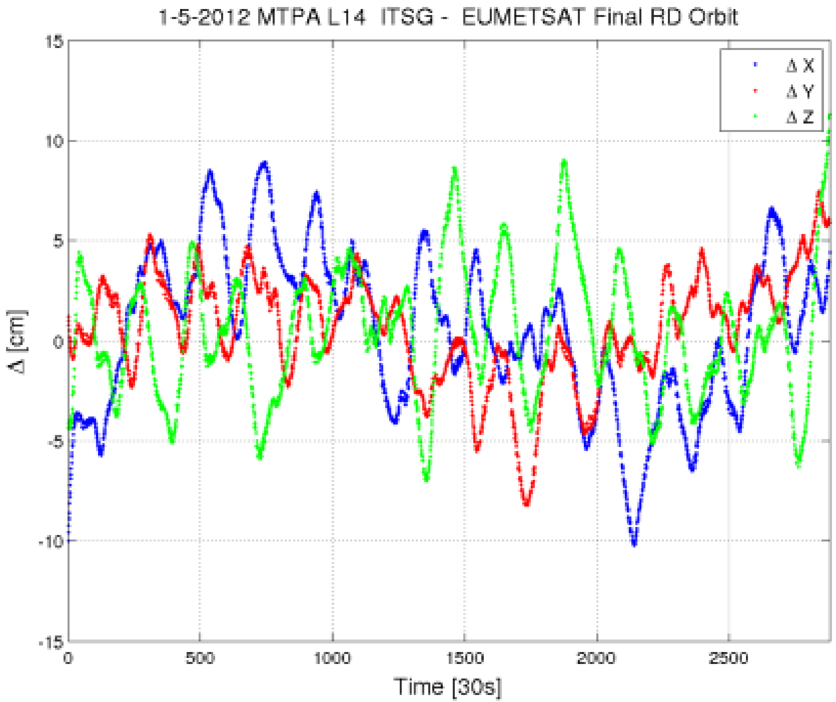
- Overview of the Bernese-part processing flow for daily LEO orbit arcs



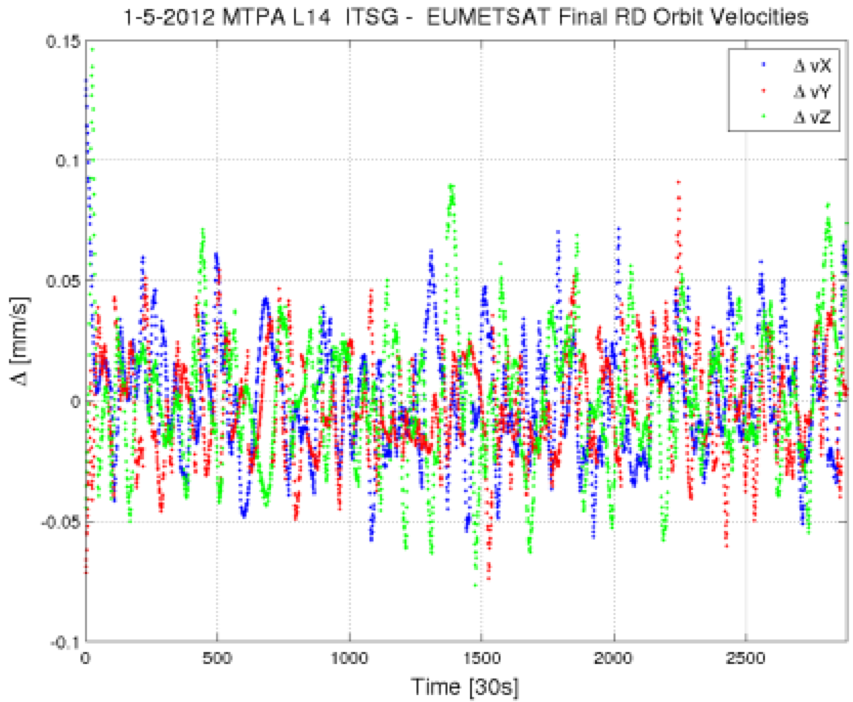
rOPS (2b) – bgr sys modeling example - LEO Rx system



- **Question:** Is processing strategy appropriate? → YES
- **Analysis Center: EUM; MetOp-A → Napeos EUM vs Bernese WEGC**



	[min]	[max]	[mean]	[rms]
dX [cm]	-10.20	8.90	0.52	3.97
dY [cm]	-8.20	7.40	0.60	2.78
dZ [cm]	-7.00	11.30	0.40	3.26



	[min]	[max]	[mean]	[rms]
dvX [mm/s]	-0.06	0.13	0.00	0.02
dvY [mm/s]	-0.07	0.09	0.00	0.02
dvZ [mm/s]	-0.08	0.15	0.00	0.03

rOPS (3) – some essential processor design aspects

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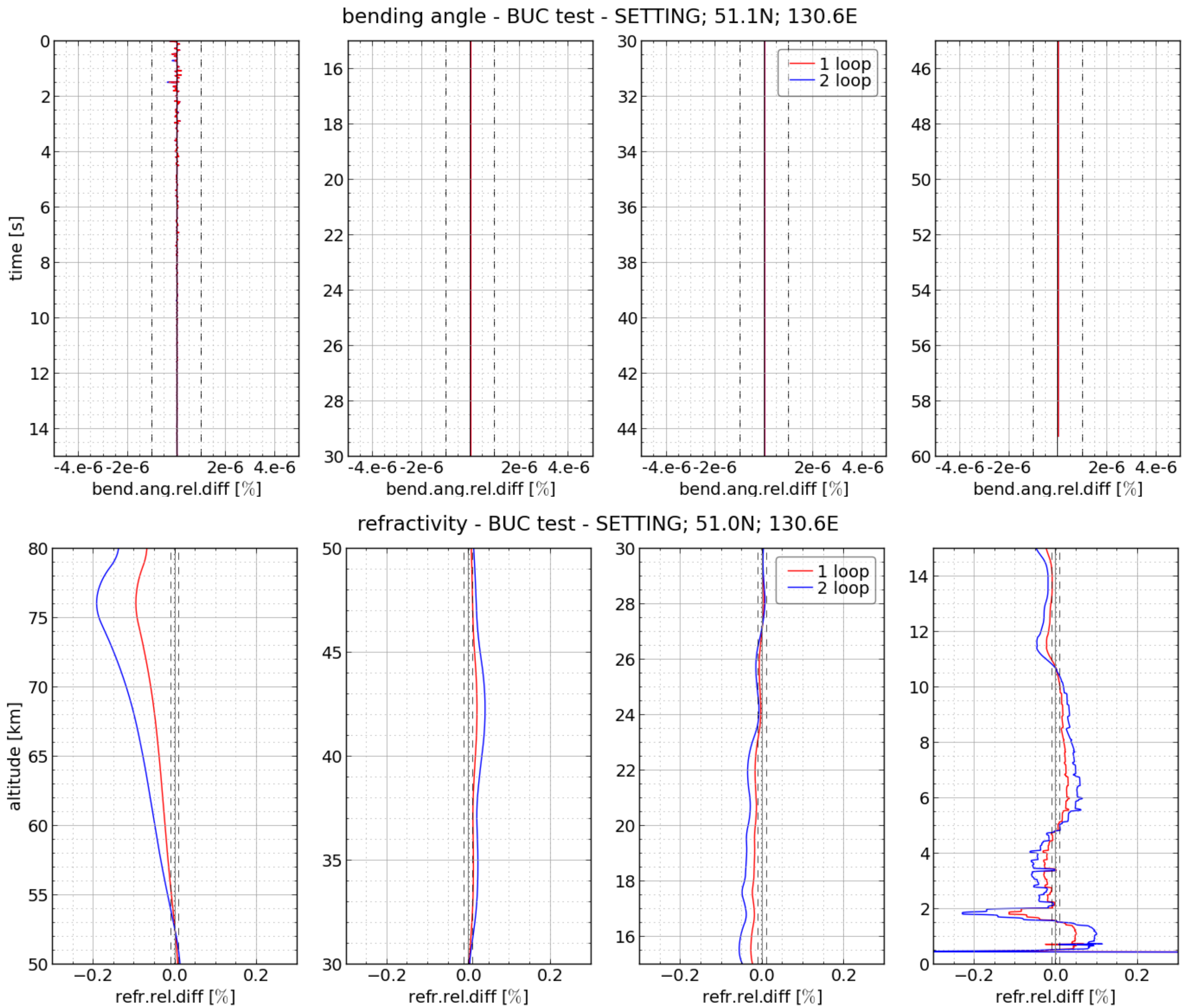
Four guiding principles for the data processing design:

- Baseband approach: L1b/L2 data processing (state retrieval, associated uncertainty estimation, and QC) mainly done on delta-profiles obtained from "down-conversion" with L1, L2 data models (e.g. $\delta\boldsymbol{x}_{\mathrm{rm}}=\boldsymbol{x}_{\mathrm{r}}-\boldsymbol{x}_{\mathrm{m}}$); pros: low dynamic range, minimized biases, simplified operators, etc.
- Forward-inverse consistency and reversibility: vertical grid model ($z \rightarrow z_p$, z_a, $a_z \leftrightarrow a_t$, z_{at}, z_t, $t^{\mathrm{s}}_t \leftarrow t$) and fwd-inv process operators ($\varphi(t) \leftrightarrow d(t) \leftrightarrow \alpha(a) \leftrightarrow N(z) \leftrightarrow p_{\mathrm{d}},T_{\mathrm{d}} \leftrightarrow p,T,q$) consistent and reversible within tight constraints ($\Delta x/x < 10^{-6}$ to 10^{-4}); pros: negligible num.residual errors, etc.
- Integrated uncertainty estimation: given the baseband approach and simple linear (matrix-algebraic) process operators, forward and inverse uncertainty propagation ($\boldsymbol{u}^{\boldsymbol{s}}_{\mathrm{x}}$, $\boldsymbol{u}^{\boldsymbol{c}}_{\mathrm{x}}$; $\boldsymbol{R}_{\mathrm{x}}$; $\boldsymbol{w}_{\mathrm{x}}$) comes in seamless and is fast; pros: rigorous QC'ed uncertainty trace, explicit vertical resolution, etc.
- Increased processing speed: given the smart(er) rOPS design and "optimally coded" core modules, aim at increased L1b/L2 processing speed (vs OPSv5.6), despite much higher rOPS information content.

Use this new and more capable design also for improved component algos…

rOPS (3a) – fwd/inv consistency examples - $d(t),\alpha(a),N(z)$



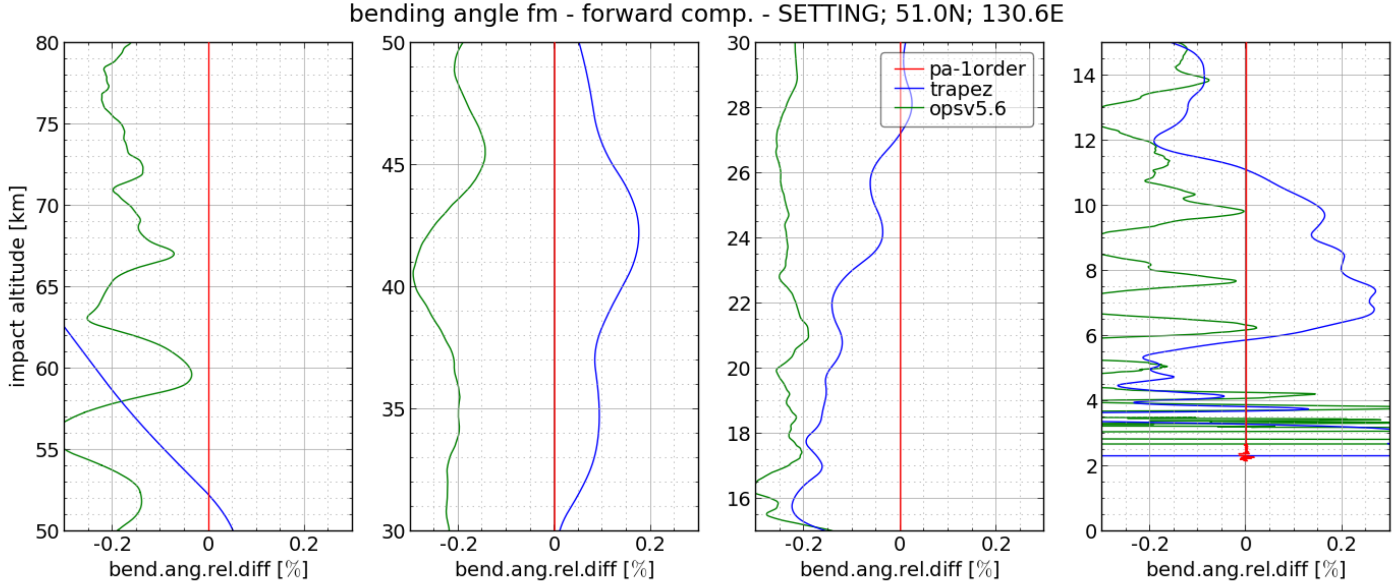
$d(t^s_t) \leftrightarrow \underline{\alpha(a_t)}$

$(\Delta x/x < 10^{-6})$

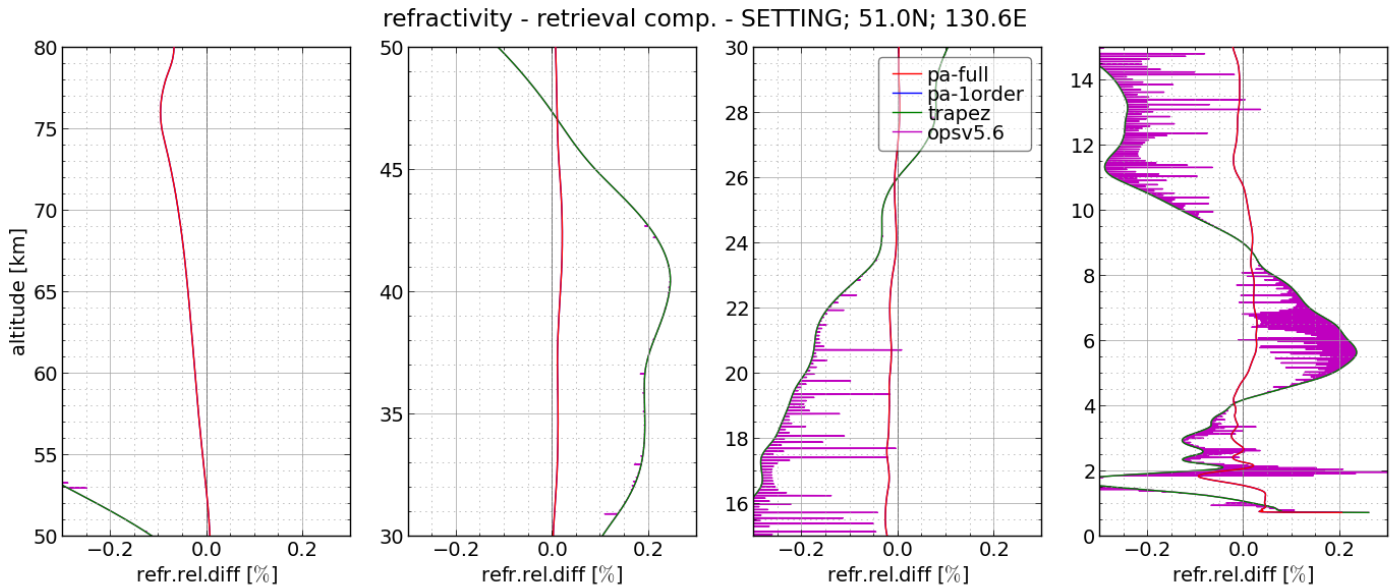
$\alpha(a_z) \leftrightarrow \underline{N(z)}$

$(\Delta x/x \sim 10^{-4})$

rOPS (3b) – fwd/inv consistency examples - $\alpha(a), N(z)$ comp

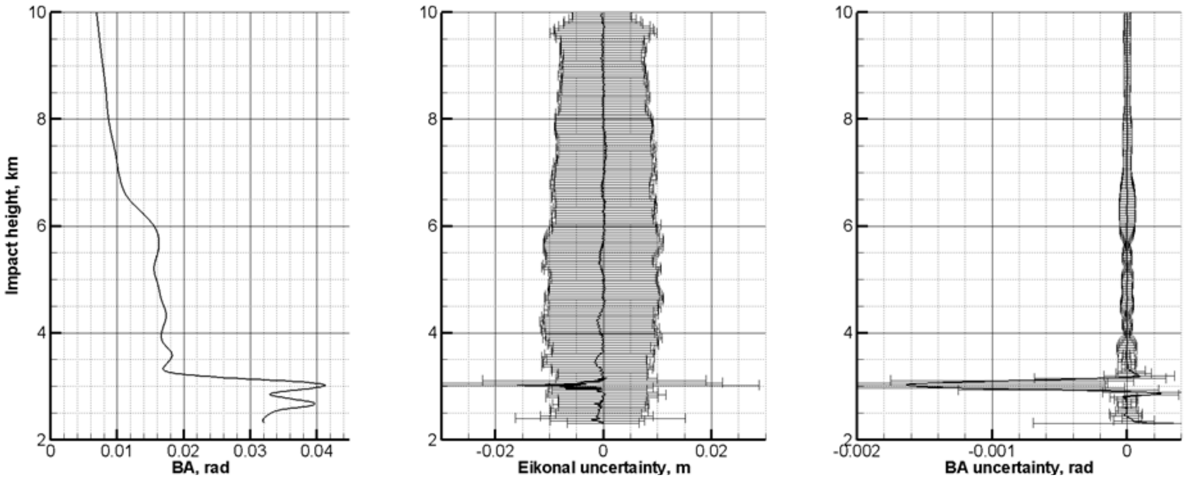


$\underline{\alpha(z_a)} \leftrightarrow N(z)$
fwd comp, vs simple trapez and opsv5.6

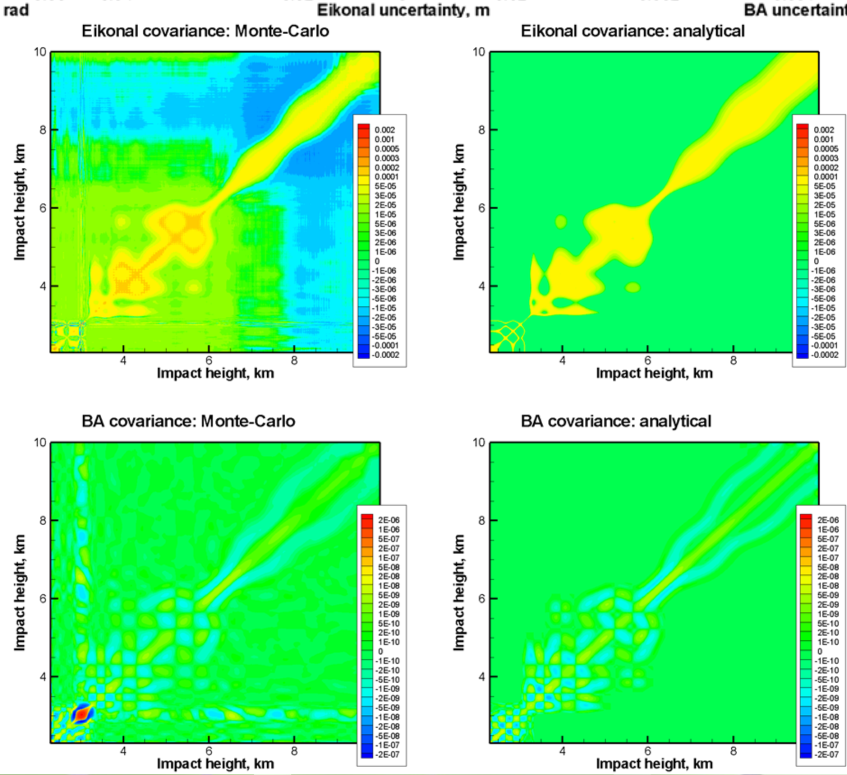


$\alpha(z_a) \leftrightarrow \underline{N(z)}$
inv comp, vs simple trapez and opsv5.6

rOPS (3c) – integrated uncert estim example - waveopt $\alpha(a)$



<u>Tropical example case</u> (from Gorbunov & Kirchengast, Uncertainty propagation through WO retrieval…, subm *Radio Sci.*, 2015)



$$u(t) = A(t)\exp(ik\Psi(t)) = \exp(ik\Sigma(t)),$$

$$\chi(t) = \ln A(t),$$

$$\Sigma(t) = S_0(t) + \Delta S(t) - i\frac{\chi(t)}{k} = \Psi(t) - i\frac{\chi(t)}{k},$$

$$\Sigma(t) = \Sigma_0(t) + \delta\Sigma(t) = \Sigma_0(t) + \Sigma_1(t) + \Sigma_2(t),$$

$$v(p) = \exp\left[ik\left(\Sigma_1(t_s(p)) + \Sigma_2(t_s(p))\right)\right]v_0(p),$$

$$v(p) = \left(\tilde{A} + \delta\tilde{A}\right)\exp\left(ik\left(\tilde{\Psi}(p) + \delta\tilde{\Psi}(p)\right)\right).$$

$$\left\langle\delta\tilde{\Psi}(p_1)\delta\tilde{\Psi}(p_2)\right\rangle = \left\langle\delta\Psi(t_s(p_1))\delta\Psi(t_s(p_2))\right\rangle.$$

$$\delta\varepsilon(p) = \delta\theta \approx \delta Y(p), \quad t_s(p) = t(Y_s(p))$$

$$\left\langle\delta\varepsilon(p_1)\delta\varepsilon(p_2)\right\rangle = \frac{\partial^2}{\partial p_1\,\partial p_2}\left\langle\delta\tilde{\Psi}(p_1)\delta\tilde{\Psi}(p_2)\right\rangle.$$

rOPS (4) – the new design supports improved algorithms

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Innovative&generalized component algorithms – Examples:

- do essentially all main QC at (L1-L2) excess phase delta-profile level
- generalized GO bend.angle retrieval/fwd.modeling, for opt.accuracy
- dynamic GO-WO bend.angle merging in upper tropo, for opt.transition
- generalized Sokolovskiy et al. (2009) iono.correction, and RIE correction
- dynamic Li et al. (2015) stat.optimization, for opt. subsequent retrieval
- filters (BWS) with quantified-BW/cutoff-freq throughout, for vert resol trace
- semi-analytic solutions of Abel and hydrostatic integrals, for opt.accuracy
- generalized moist-air retrieval for essentially arbitrary refrac equations, linearized around Smith-Wein dry-air state and with dynamic bgr.info
- etc… [detailed info in the “rOPS Detailed Algorithm Description (DAD)”]

These and further <u>rOPS algorithm improvements (vs OPSv5.6) aim to destill the best of RO know-how</u> learned over the last two decades, for serving the targeted bench-qual reference RO data provision as good as possible.

rOPS (4a) – retrieval algo examples - L1b $\alpha(z_a)$ retrievals

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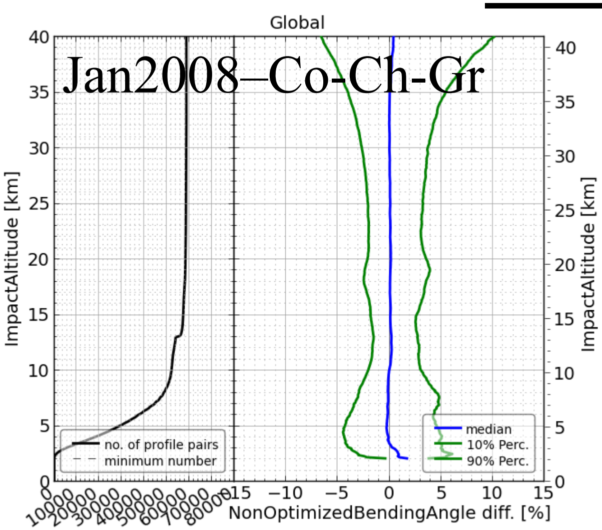
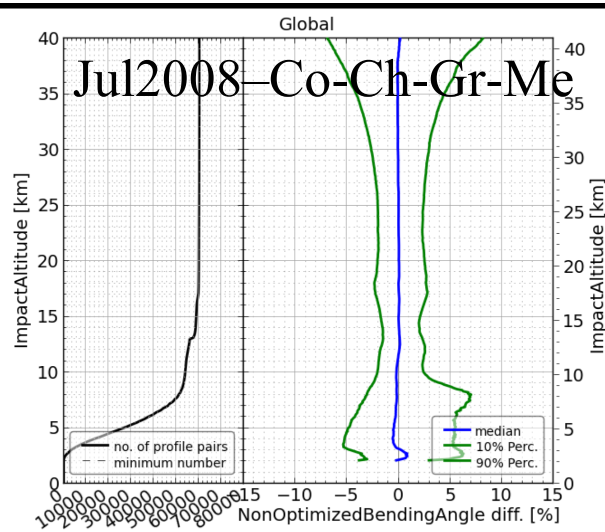
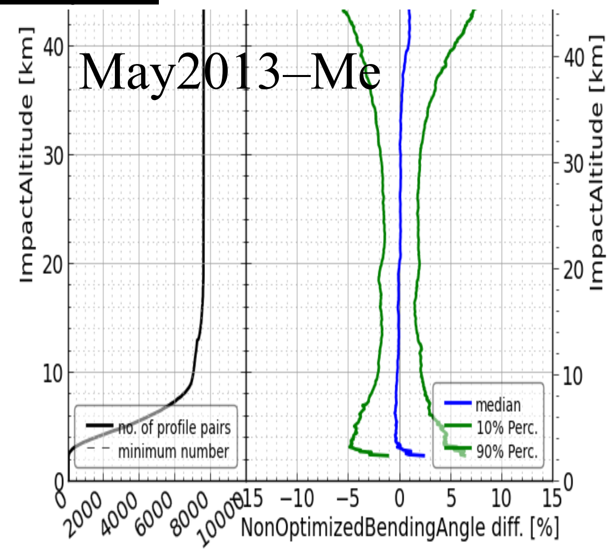
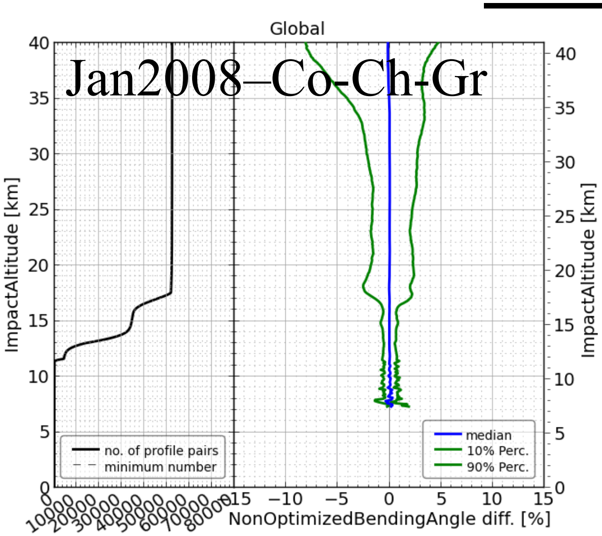
Multi-sat statistics rOPSv1 retrievals vs. ECMWF analyses for 3 test months

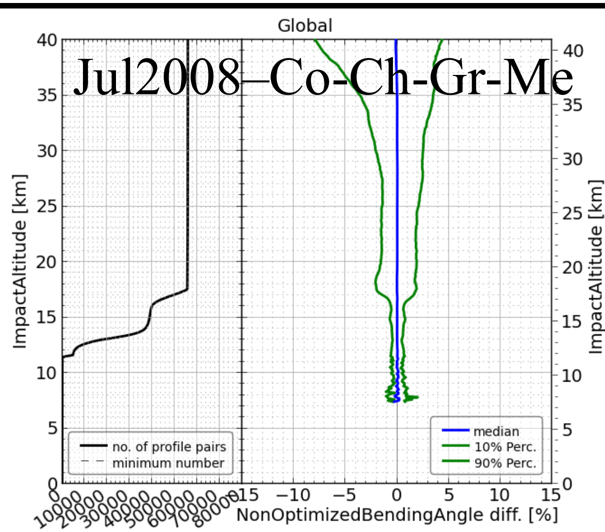


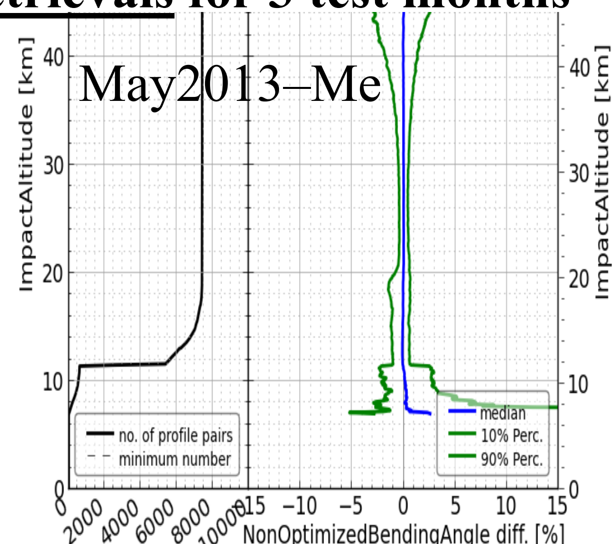




Multi-sat statistics rOPSv1 retrievals vs. OPSv5.6 retrievals for 3 test months



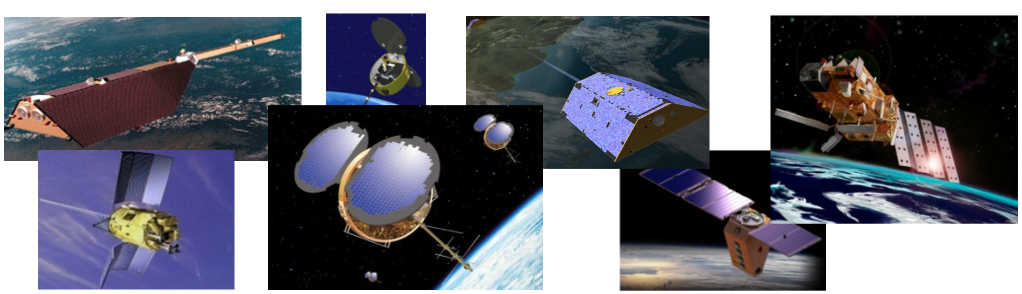




so rOPS looks useful – let's sum up and see what's next

Conclusions and Prospects:

- WEGC's rOPS is a fresh RO processing system aiming to help solve the climate monitoring problem in the free atmosphere for thermodynamic core ECVs, by providing SI-tied atmospheric profiling of these ECVs with integrated uncertainty estimation.
- In terms of research and applications, the key use is benchmark-quality reference RO data provision for calibration/validation and for climate monitoring, research, and services, complementary to NRT.
- rOPS, developed as v1 over 2011 to 2015, will replace WEGC's OPSv5 processing system operating over 2007-2015 (following EGOPSv2-v4/ CCRv2 heritage of 1996-2006). OPSv5.6, which just completes RO re-processing over 2001-2014, is nominally the final OPSv5 data version.
- rOPS will be published in a set of papers over 2015-2016 — stay tuned!



Thank You! ☺