

On the assimilation of GNSS radio occultation data at DWD

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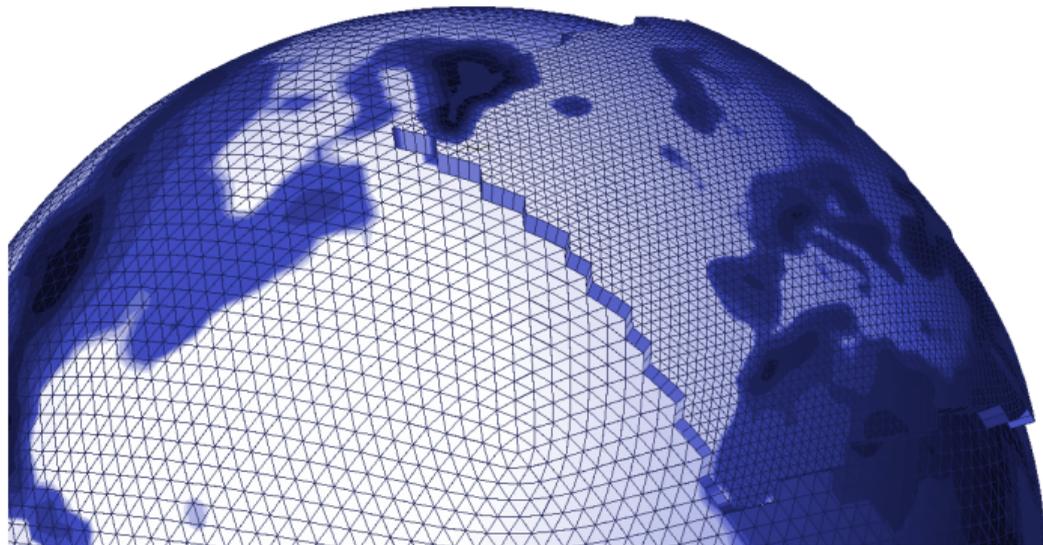
Research and Development – Data Assimilation and Predictability
Deutscher Wetterdienst, Offenbach, Germany

8th EUMETSAT ROM SAF user workshop on GNSS radio occultation measurements
ECMWF, Reading, UK, 11–13 June 2024



NWP at DWD: **ICON**-Model

- **ICO**sahedral-triangular (Arakawa C) grid, **Non**-hydrostatic core
 - ▶ Joint development by DWD (NWP) and MPI-M Hamburg (climate)
 - ▶ unstructured mesh, local refinement, (self-)nesting (horiz./vertical, 1-/2-way)
- Global NWP operational configuration
 - ▶ det: 13 km @ 120 layers
 - ▶ ens: 26 km @ 120 layers ($\times 40$)
 - ▶ model top: 75 km
- Europe nest (2-way)
 - ▶ det: 6.5 km @ 74 layers
 - ▶ ens: 13 km @ 74 layers
 - ▶ top: 23 km
- For ROMEX experiments:
 - ▶ det: 26(13) km @ 120(74)
 - ▶ ens: 40(20) km @ 120(74)



Global Data Assimilation

- Hybrid Variational / Ensemble Data Assimilation

- ▶ Deterministic analysis: Ensemble-variational (“3D-EnVar”), 3-h cycle; PSAS-scheme; background error covariance

$$\mathbf{B} = \alpha \mathbf{B}_{\text{EnKF}} + (1 - \alpha) \mathbf{B}_{\text{clim}} \quad (\text{currently: } \alpha = 0.7)$$

- ★ \mathbf{B}_{clim} : climatological \mathbf{B} matrix of 3D-Var

- ★ \mathbf{B}_{EnKF} : background ensemble covariances (localized in model-space)

- ▶ Ensemble analysis: **L**ocal **E**nsemble **T**ransform **K**alman **F**ilter (LETKF)

- ★ Localization in observation space (Hunt et al., 2007)

- Radio Occultation observation operator

- ▶ Based on original code by Michael Gorbunov
- ▶ 1-d Abel integral, tangent-point drift not used operationally

Operationally assimilated GNSS-RO missions

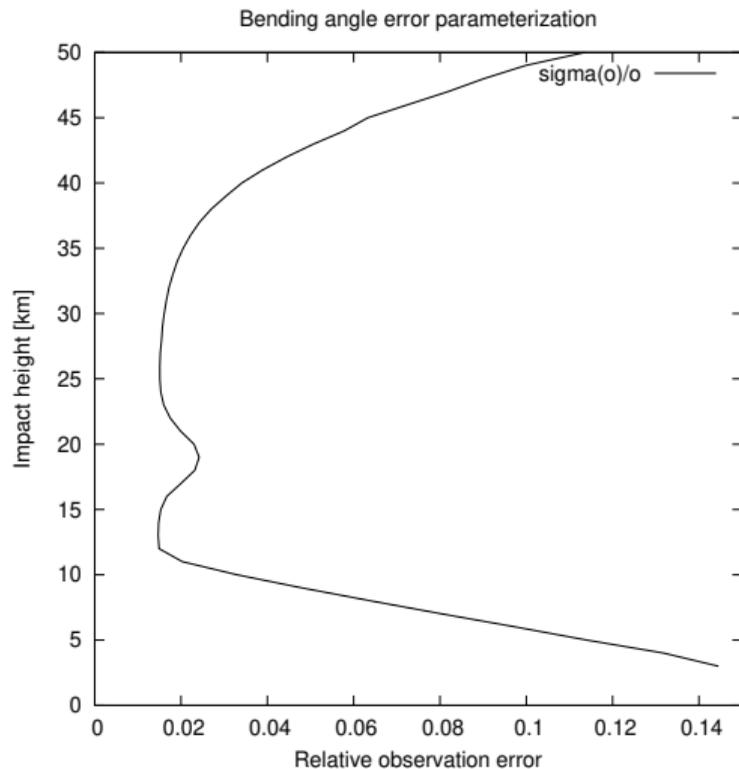
- Current (or past):
 - ▶ Metop
 - ▶ SPIRE/EUM (purchased and processed by EUMETSAT);
SPIRE/NOAA or PlanetiQ/NOAA (processed by EUMETSAT)
 - ▶ COSMIC-2; Kompsat-5, PAZ (UCAR)
 - ▶ TerraSAR-X, TanDEM-X; GRACE-C/D (GFZ)
 - ▶ FY-3D (blacklisted above 35 km)
 - ▶ Sentinel-6A/JPL (still blacklisted above 35 km, will get updated)
- Planned:
 - ▶ FY-3E

GNSS-RO Observation preprocessing

- BUFR vertical sampling of GNSS-RO profiles differs between centers
 - ▶ Also different smoothing applied before sampling, unknown to users
 - ▶ Smoothing implies correlated data errors
- NWP model vertical resolutions may differ vastly from sampling
 - ▶ Representativity of model levels? (Cannot represent structures finer than $2\Delta z$)
 - ▶ Need to:
 - ★ take into account correlation of observation error
 - ★ and/or inflate observation error
 - ★ and/or thin data
 - ▶ Super-obbing of data!
 - ★ roughly determined/guided by model vertical resolution
 - ★ partially absorbs poorly known error correlations
 - ★ allows for smaller inflation factors
 - ★ effective tangent point from lower part of profile
 - ★ but: may be problematic in lower troposphere where larger gradients are to be expected

GNSS-RO Observation error model

- Normalized (relative) observation error: σ_o/O
- Parametric ansatz, with contributions:
 - ▶ (Stratospheric) noise floor
 - ▶ Ionospheric residual
 - ▶ Tropospheric variability, representativeness
 - ▶ Additional term to mimic:
 - ★ Representativeness (e.g. near tropopause)
 - ★ or processing artifacts (e.g. transition GO/WO processing)
- Simple, smooth dependence on $\cos(\text{latitude})$
- Optionally: GNSS, processing center
- Coefficients derived using Desroziers method (with subjective adjustments/inflation)



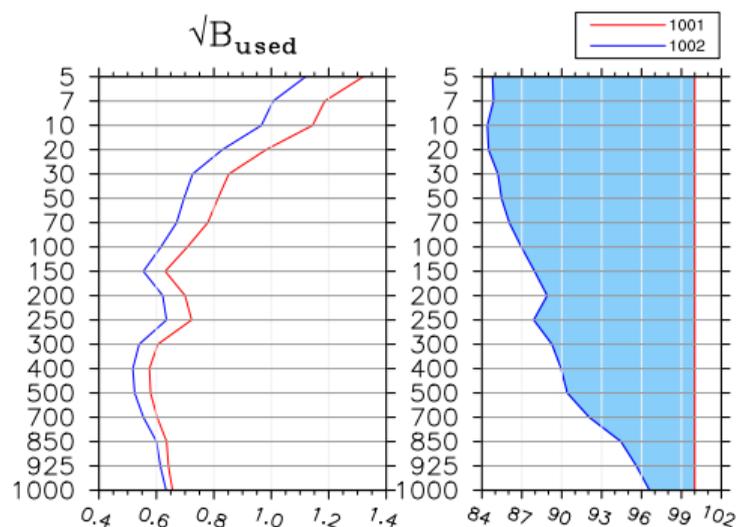
Data selection, Quality control

- Impact height range used: 3-50 km
- General QC settings for RO
 - ▶ Dismiss profiles flagged by provider
 - ▶ Standard first-guess checks (e.g. $|O - B| < 3\sqrt{\sigma_o^2 + \sigma_b^2}$)
 - ▶ Upper bound on bending angle: 30 mrad
 - ▶ Reject data up to 250 m above model super-refraction layers
 - ▶ Reject data where background vertical refractivity gradient exceeds 0.5 times critical value
 - ▶ Reject profiles with more than 30 % rejected rays
 - ▶ Inflate observation error so that σ_b/σ_o does not exceed 2 (see also example later below)
- Partial blacklisting of profiles based on monitoring
 - ▶ e.g. Metop rising below 5 km: FY-3D above 35 km

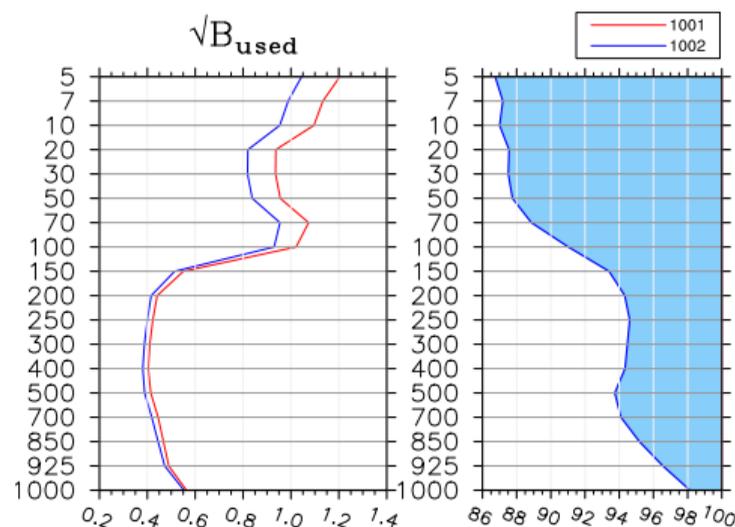
- **R**adio **O**ccultation **M**odeling **EX**periment
- Purpose: demonstrate impact of large numbers of real RO data on NWP models
 - ▶ including all public and many commercial satellites/constellations
 - ▶ ROMEX-1 common period: Sep-Nov 2022
 - ▶ “experiment”: $\sim 35\text{k}$ profiles/d
 - ▶ “baseline”: $\sim 7\text{k}$ profiles/d
- Intermediate results at EUMETSAT ROMEX Workshop, Darmstadt, April 2024
- Comparison against independent observations (e.g. radiosondes):
 - ▶ Overall impact considered positive, but some concern due to not yet fully resolved deterioration of some verification scores against radiosondes at shorter leadtimes
 - ▶ Increase (by $\approx -0.1\text{ K}$) of slight cold lower tropospheric bias observed with ICON
 - ▶ Systematic change e.g. in mean lower tropospheric temperature seen by several groups (e.g. DWD, ECMWF, MeteoFrance, KMA, GFS), shift in geopotential height
- Subsequent sensitivity tests done by several groups (e.g. ECMWF, MetOffice)

ROMEX: Impact on background ensemble spread

- 3-h forecast spread of **temperature** at radiosonde locations:
 - ▶ NH spread reduction: 10–15 % in upper troposphere/stratosphere; 5–10 % in the troposphere
 - ▶ Height-dependence qualitatively consistent with expected RO impact
 - ▶ Impact in tropical troposphere significantly lower (of order 5 %)



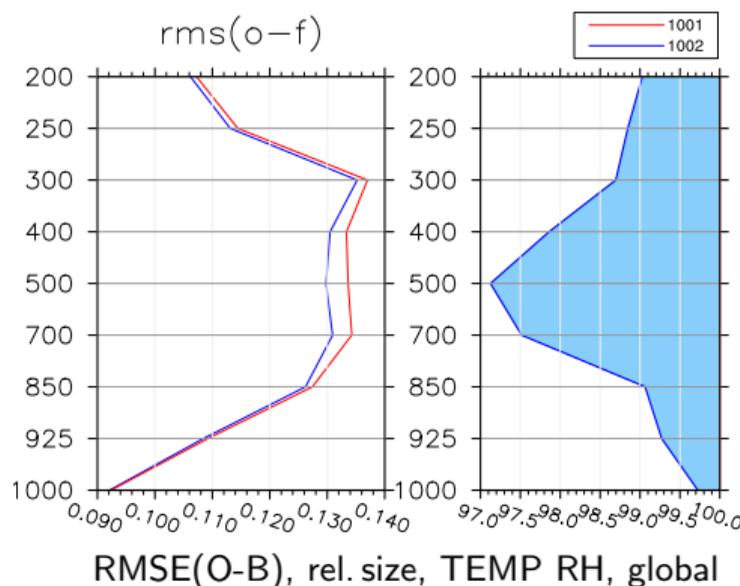
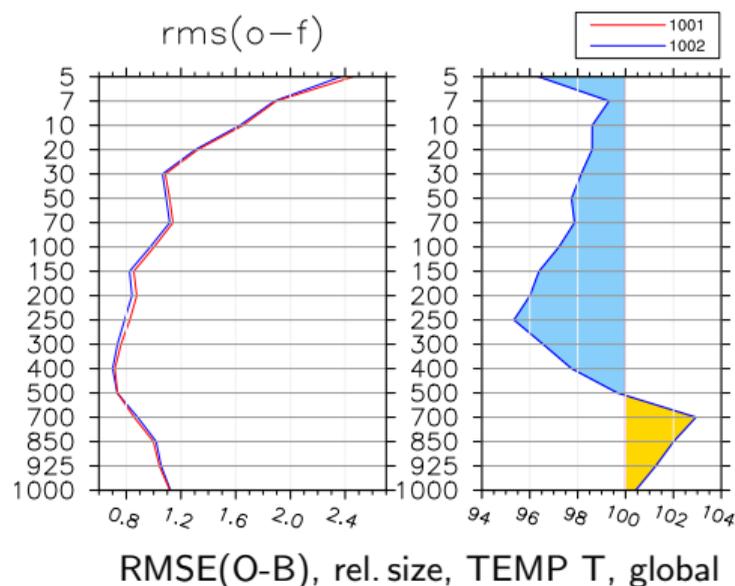
Ensemble T spread, Northern Hemisphere



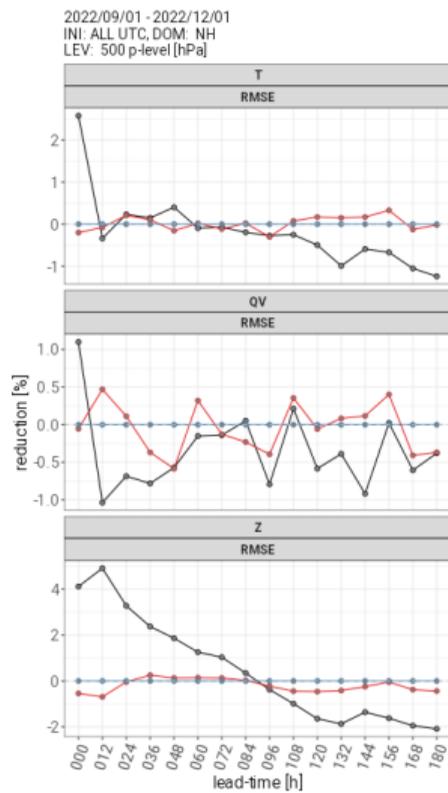
Ensemble T spread, Tropics

ROMEX: Assimilation cycle, fit to radiosondes

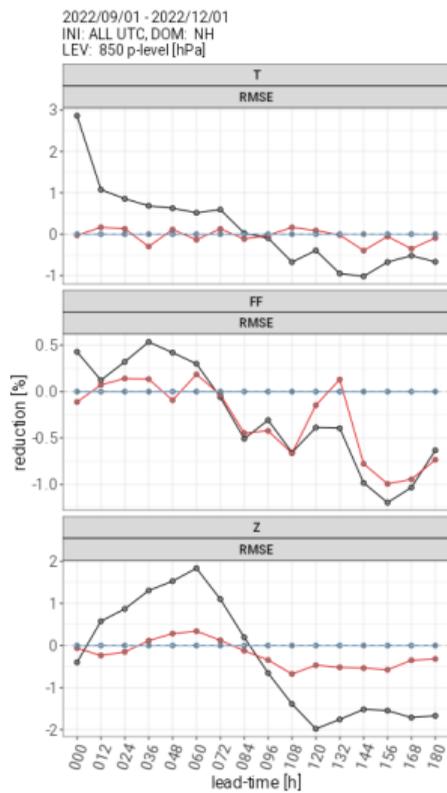
- RMSE of det. 3-h forecast against radiosondes:
 - ▶ Reduction of **temperature** error up to 4% (UTLS), but degradation in lower troposphere!
 - ▶ Reduction of **rel. humidity** error up to 3% in mid-troposphere
 - ▶ Fit of ensemble 3-h forecasts very similar (not shown)



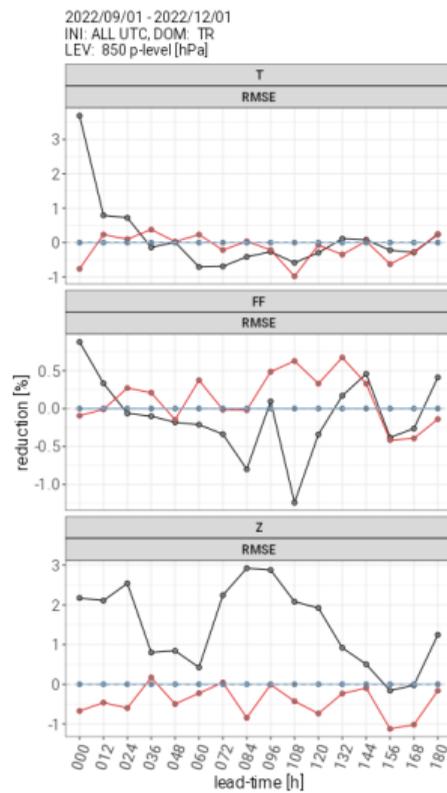
ROMEX: preliminary TEMP verification examples, norm. RMSE(FC-O)



NH, 500 hPa



NH, 850 hPa



TR, 850 hPa



Remarks on DWD's RO observation operator implementation

- Refractivity: Aparicio and Laroche, JGR 116 (2011)

$$N \simeq N_0 \left(1 + N_0 \cdot 10^{-6}/6\right), \quad N_0 = \rho_d \cdot (b_1 + b_2/T) + \rho_w \cdot (b_3 + b_4/T) \quad (1)$$

ρ_d, ρ_w : densities of dry air and water vapor. (Uncertainty of coefficients b_i not given.)

- Non-ideal gas effects

- ▶ Density of moist air: CIPM-2007 (Picard et al., Metrologia 45 (2008) 149)

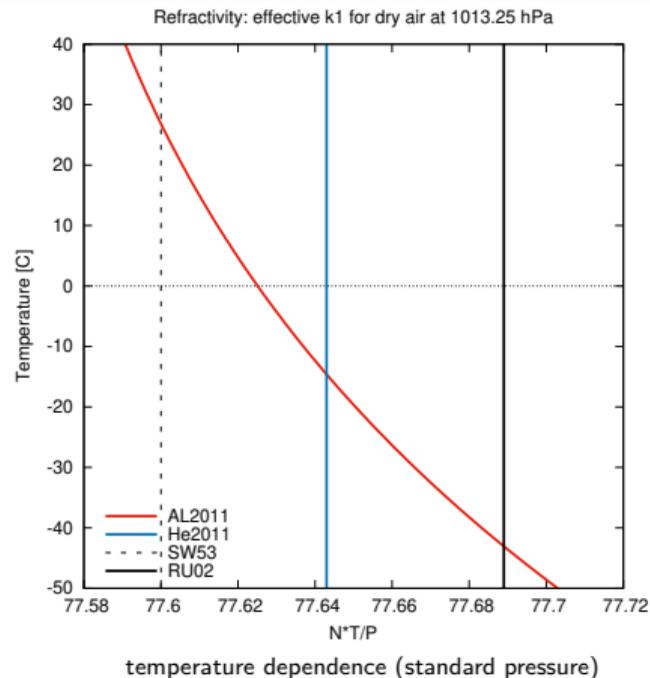
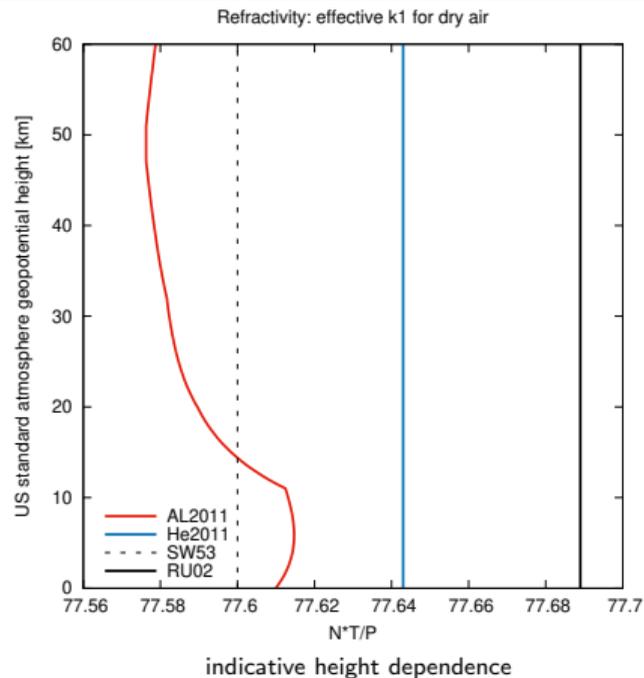
$$\rho = \frac{p}{R_d T_v}, \quad T_v = T \cdot \left[1 + q \left(\frac{M_d}{M_v} - 1\right)\right] \cdot Z, \quad Z = Z(T, q) \quad (2)$$

- ▶ Hydrostatic integration in observation operator (to be converted to geometric altitude):

$$h = - \int \frac{R_d T_v}{g} \frac{dp}{p} \quad (3)$$

Comparison of refractivity expressions: dry air, normalized

- (NT/P): US Standard Atmosphere profile (sea level: 15°C); temperature dependence
 - ▶ Aparicio & Laroche (2011), Healy (2011), Smith-Weintraub (1953), Rieger (2002)

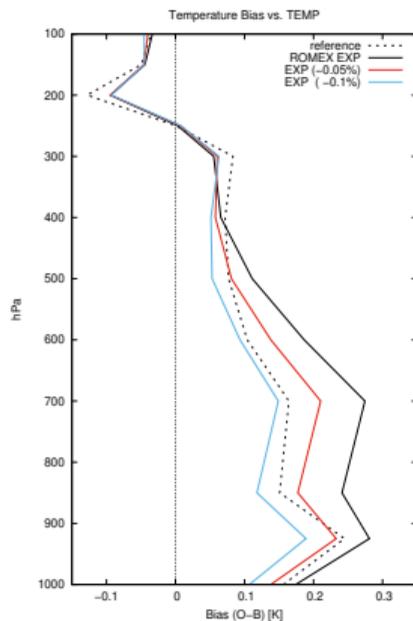


Uncertainty of refractivity expressions

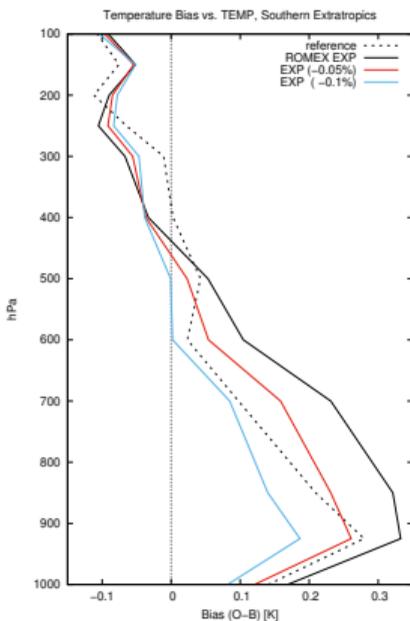
- Differences between refractivity expressions (e.g. Healy 2011, Aparicio & Laroche 2011)
 - ▶ Overall variation ($\sim 0.1\%$) larger than accuracy quoted for experimental results ($< 0.05\%$)
 - ▶ Current status of literature may not give a clear indication what to use
 - ▶ See also Aparicio & Laroche, MWR D14 (2015) 1259 for impact studies
- Is a physically motivated parameterization to prefer over a naive fit to data?
 - ▶ In theory: yes
 - ▶ But every fit should come with an uncertainty estimate
 - ▶ Can we specify realistic uncertainty estimates for each parameterization in use? (incl. Aparicio & Laroche)
- How relevant is the uncertainty for data assimilation in NWP?
 - ▶ Tests in DA systems with low number of RO may underestimate the significance
 - ▶ Assessment of impact by large numbers of RO profiles \implies ROMEX

Sensitivity test to changes in refractivity expression

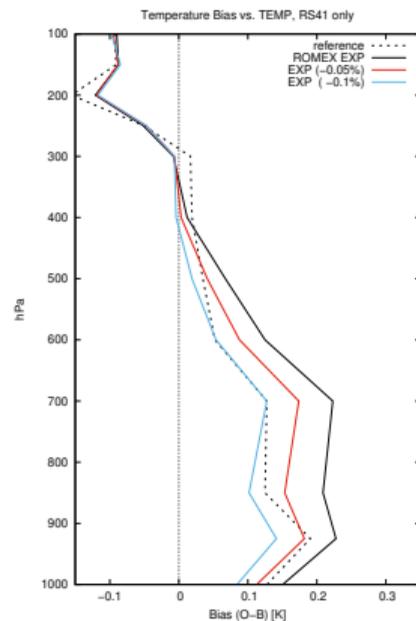
- Bias of 3h forecasts against radiosonde **temperature**, September 2022
 - ▶ Reference (= baseline) vs. EXP (AL2011 coeffs. / -0.05% / -0.1%)



global



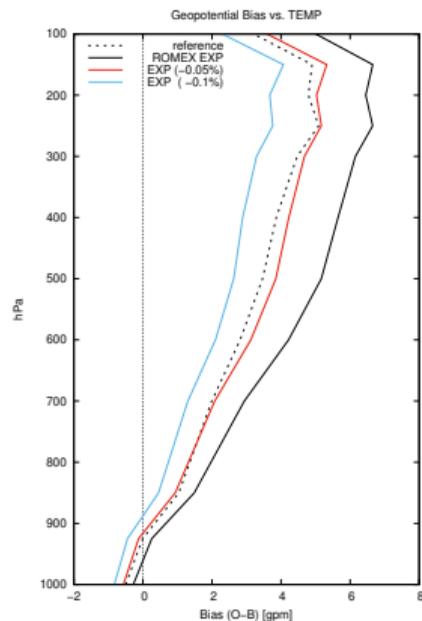
Southern Hemisphere



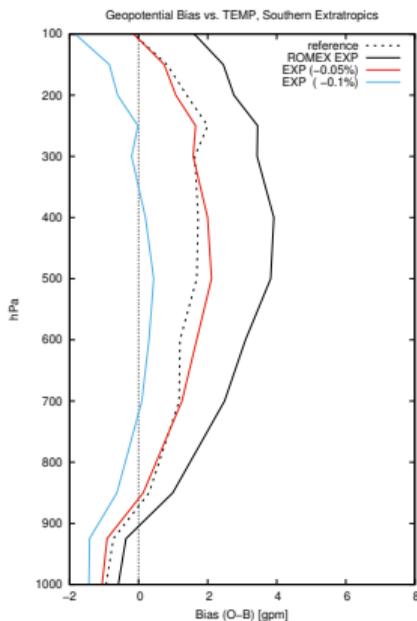
global, vs. RS41-only

Sensitivity test to changes in refractivity expression

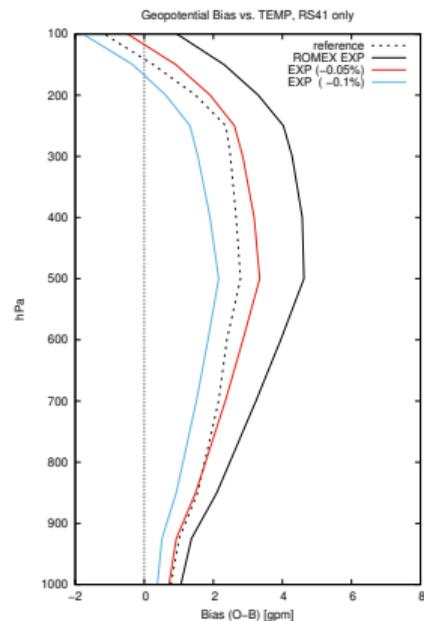
- Bias of 3h forecasts against radiosonde **geopotential height**, September 2022
 - ▶ Reference (= baseline) vs. EXP (AL2011 coeffs. / -0.05% / -0.1%)



global



Southern Hemisphere



global, vs. RS41-only

Remarks and some questions

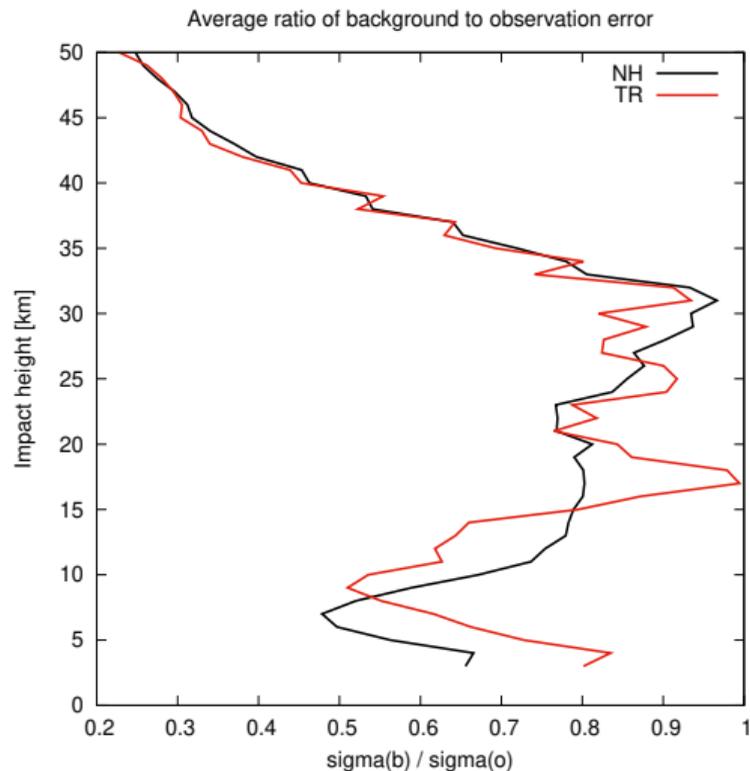
- Radiosondes are a common (more or less absolute) reference in NWP
 - ▶ Quality does differ between different RS types!
 - ★ see e.g. WMO's 2022 Upper-Air Instrument Intercomparison Campaign
 - ▶ Geopotential height
 - ★ Method of derivation from GPS height prescribed by WMO (Guide to Instruments and Methods of Observation, Section 12.5.5.2)
 - ▶ How much trust in consistency of reported profiles (geopotential height vs. temperature)?
 - ★ use e.g. RS41 as reference?
 - ★ or only use GRUAN sites?
- Model climate should ideally **not** depend on number of assimilated observations
 - ▶ when to adjust observation operator or to use a bias correction?
 - ▶ caveat: NWP system has not been tuned otherwise; we may have met a latent problem!
- Recommendations?

Biases in data assimilation

- Some possible causes for biases of analyses
 - ▶ Model background systematically affected by model issues
 - ▶ Feedback between data assimilation and model (physics)
 - ★ e.g. change in tropospheric vertical temperature gradient influences convective activity
 - ★ e.g. spin-up/-down, can be studied only in a cycled system (DA + model)!
 - ▶ Issues in observations operators (see above)
 - ▶ Systematic differences in $(O - B)$ may be caused by biased observations
 - ★ example: rising/setting differences clearly caused by observations or processing
 - ★ biases seen mostly at low or high impact heights
 - ★ can be dealt with by partial blacklisting of data
- Relevance of bias in $(O - B)$?
 - ▶ Depends on assimilation system, background error (σ_b), assigned observation error (σ_o)
 - ▶ A bias at one height can alias into increments at different heights (Jacobian, \mathbf{B} matrix)
 - ▶ What if the bias is seen against an anchor system (Radiosonde, RO)?

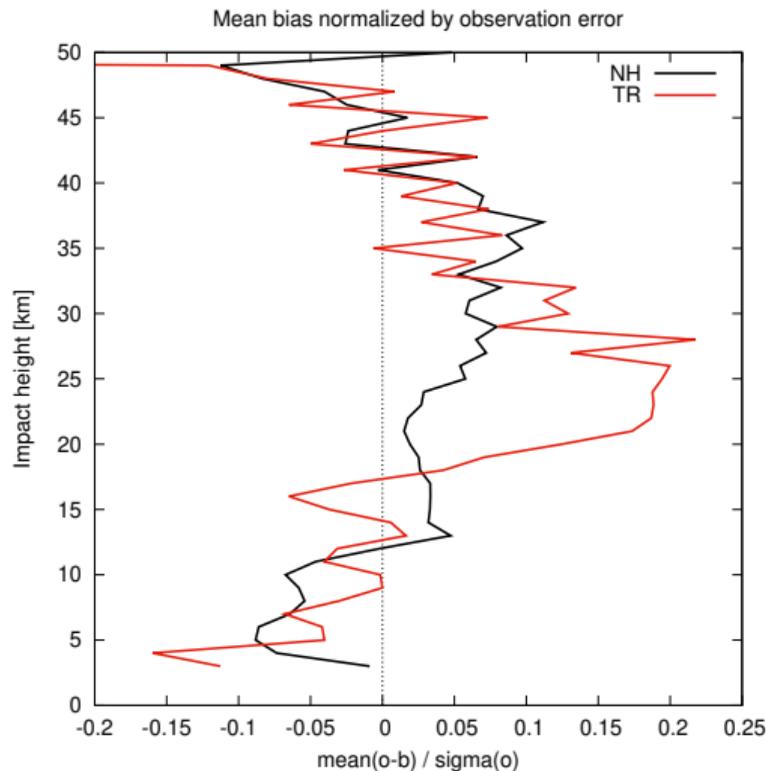
Gross estimate of average RO impact

- Background error σ_b mostly smaller than assigned observation error σ_o
- The higher the ratio $(\sigma_b/\sigma_o)^2$, the higher the expected (local) impact
- For DWD's system, the expected impact in the lower troposphere is higher in the tropics than in the extra-tropics (also with tuning of observational error)
- Note: σ_o is assumed situation-independent, while σ_b is situation-dependent (EnVar!)



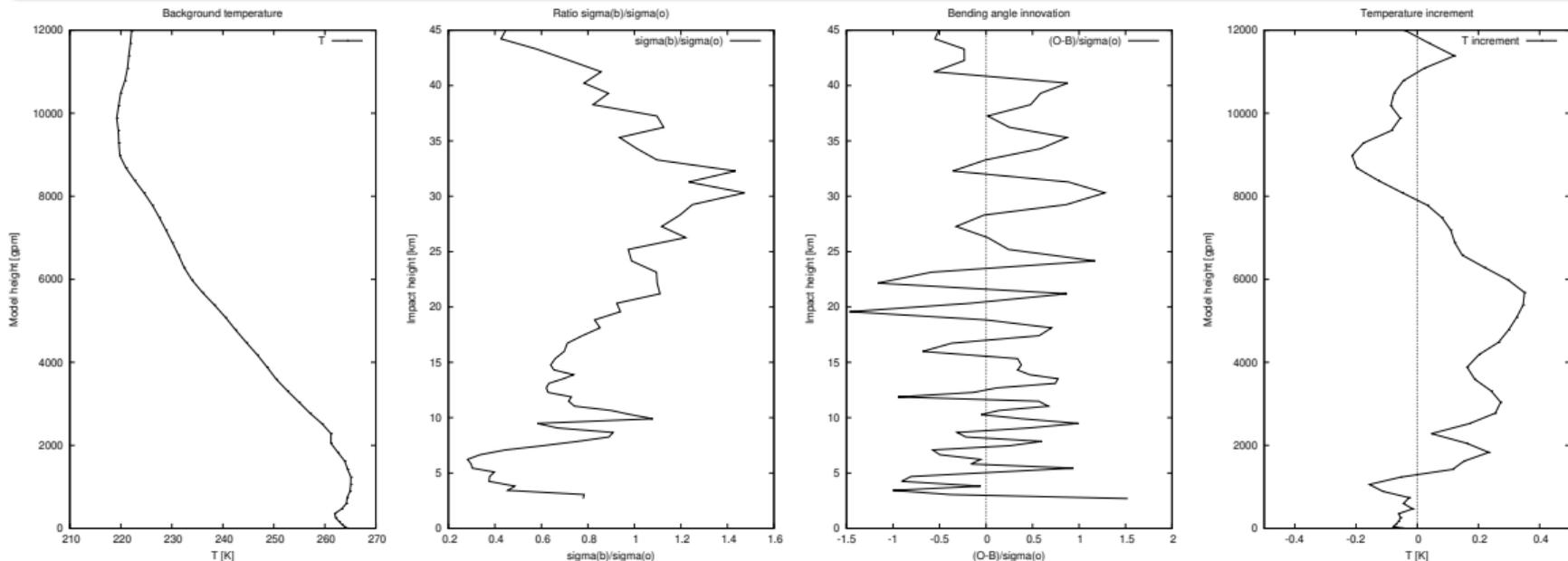
Mean bias of model against RO

- Bias normalized by observation error σ_o
 - ▶ Active observations only
- Bias mostly small
 - ▶ Model bias likely in tropical stratosphere
- Negative bias in mid- to lower troposphere seen for several missions
 - ▶ Varies between satellites/processing
 - ▶ Blacklist below empirical height (e.g. Metop rising below 5 km)



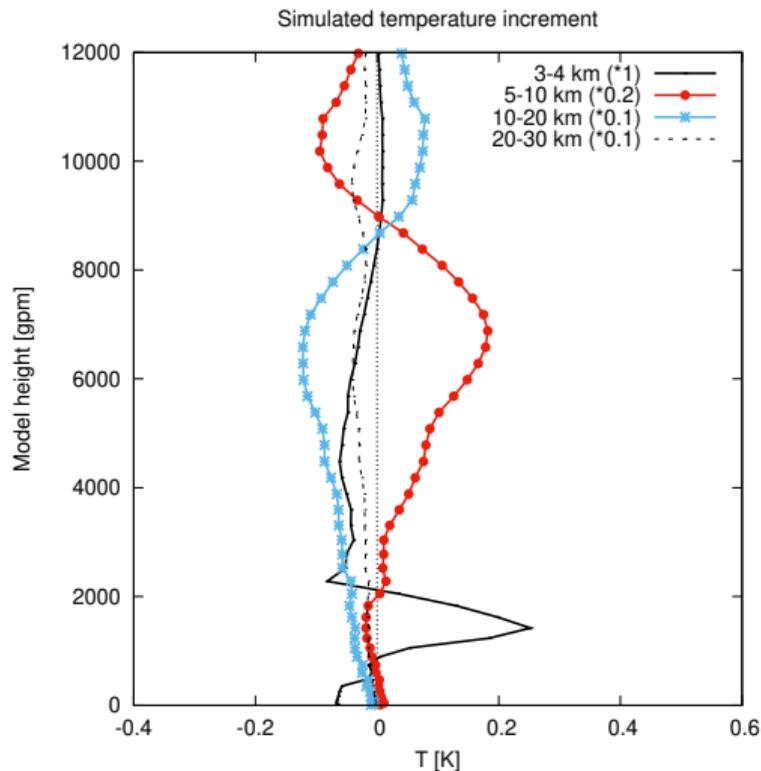
Situation dependence – a mini study - case 1

- Case 1: a “normal” profile at high latitudes (2023-12-09 04:39Z, near 60.5°N/88°W)
 - ▶ Near-surface inversion, although below lowest assimilated bending angle
 - ▶ Very moderate increments in lower troposphere



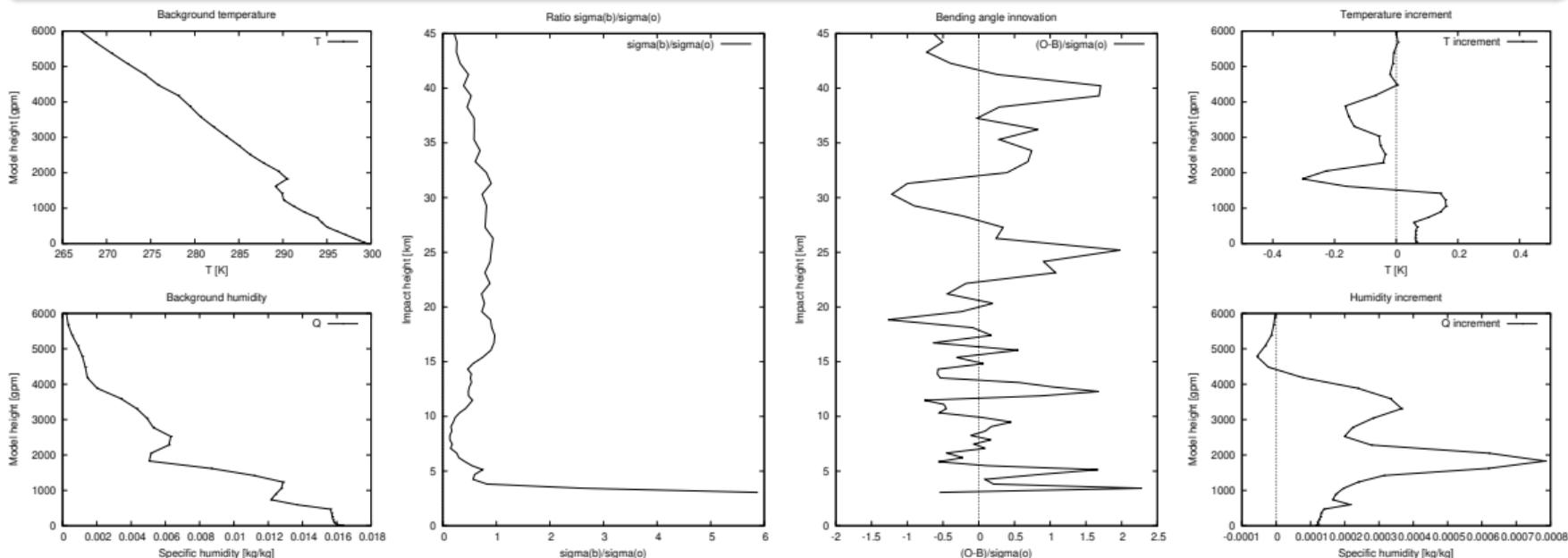
Situation dependence – a mini study - case 1

- If there were a bias $O - B$ over a **limited** height range, how would corresponding analysis increments look like?
- Simulate temperature increments for fixed $O - B$ in a height range:
 - ▶ $(-1) \cdot \sigma_o$ between 3-4 km
 - ▶ $(-0.2) \cdot \sigma_o$ between 5-10 km
 - ▶ $(-0.1) \cdot \sigma_o$ between 10-20 km
 - ▶ $(-0.1) \cdot \sigma_o$ between 20-30 km
- Moderate biases in lower to mid-stratosphere can lead to small (but smooth!) temperature increments in the lower troposphere



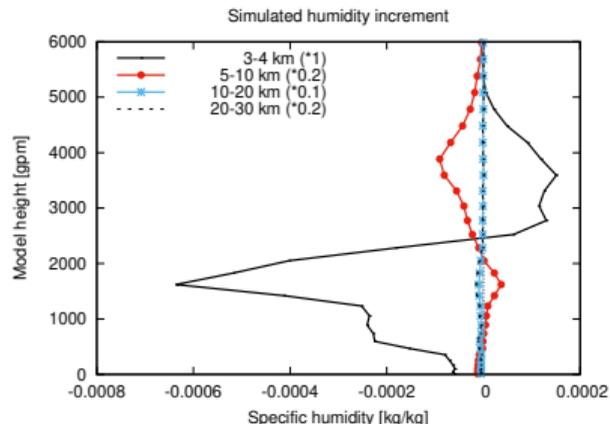
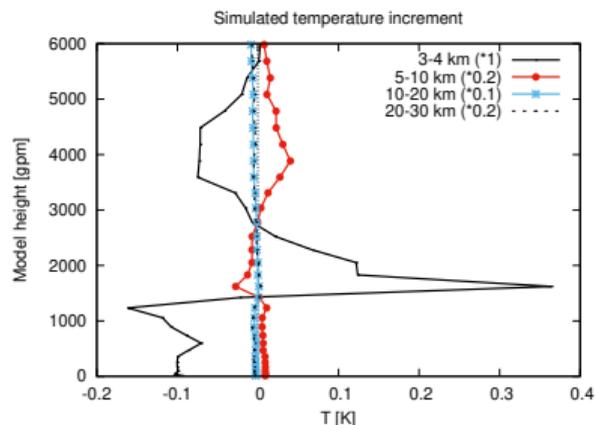
Situation dependence – a mini study - case 2

- Case 2: a profile in the tropics (2023-12-09 06:34Z, near 5°S/26.5°W)
 - ▶ Inversion near 2 km a.s.l., background close to super-refraction below 3 km impact height
 - ▶ Large dynamic background error (contribution of ensemble covariance!)



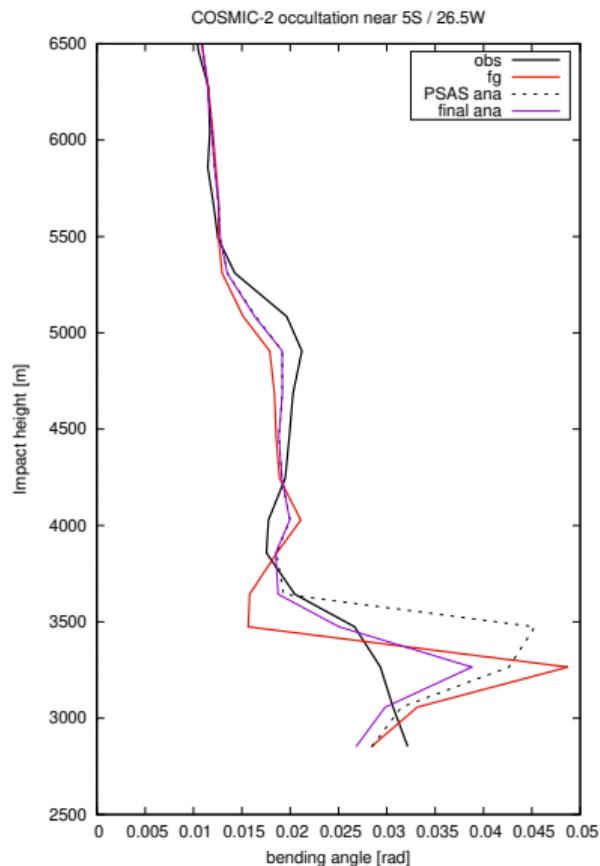
Situation dependence – a mini study - case 2

- Again, assume a representative bias over a limited height range
- Simulate temperature increments for fixed $O - B$ in a height range:
 - ▶ $(-1) \cdot \sigma_o$ between 3-4 km
 - ▶ $(-0.2) \cdot \sigma_o$ between 5-10 km
 - ▶ $(-0.1) \cdot \sigma_o$ between 10-20 km
 - ▶ $(-0.2) \cdot \sigma_o$ between 20-30 km
- Moderate biases in lower to mid-stratosphere do not lead to relevant increments in lower troposphere in the present case
- A negative bias at 3-4 km would lead here to a cooling and drying below 1.5 km/ 850 hPa



Remarks

- There is nothing obviously wrong with either the observation or the model
- But case 2 is challenge to variational assimilation, esp. in presence of other observations
 - ▶ High ratio σ_b/σ_o
 - ★ very high weight given to observation
 - ★ linesearch scans through strong non-linearities
 - ▶ Convergence often slower
 - ▶ Analysis in observation space (PSAS) can differ significantly from “final analysis” (= observation operator applied to analysis)
- Is simple observation error model applicable here?
 - ▶ At least doubtful
 - ▶ Limit σ_b/σ_o by increasing σ_o !



Thoughts

- Background error is dynamical, situation-dependent
- Replace the simple, statistical observation error model by something more dynamical?
 - ▶ Predictors?
 - ▶ Can we get supporting information from processing (e.g. local spectral width, ...)?
- Would a higher vertical sampling rate of RO profiles help for assimilating into NWP models with high vertical resolution (> 100 model levels)?
 - ▶ Beyond the current 247 levels
 - ▶ With reduced smoothing by processing to allow users to test own smoothing/thinning/super-obbing

Concluding Remarks

- High impact of GNSS radio-occultation data in global NWP reconfirmed by ROMEX with high volumes of supplemental data
 - ▶ The role of GNSS-RO as an anchor system besides radiosondes will increase: global coverage, with almost uniform data quality in the core region
 - ▶ Utility may depend on quality of implemented forward models: do we need to reevaluate the accuracy of refractivity expressions etc.? (Target: uncertainties equivalent to $\ll 0.1$ K)
- The BUFR data disseminated for NWP contain ~ 247 levels since 20 years
 - ▶ NWP model vertical resolution has significantly increased over that period: Users may want to test higher-resolved vertical sampling of RO profiles
 - ▶ Is there more we can learn from higher vertical sampling?
- Exchange ideas for better modeling of observation error / situation-dependence