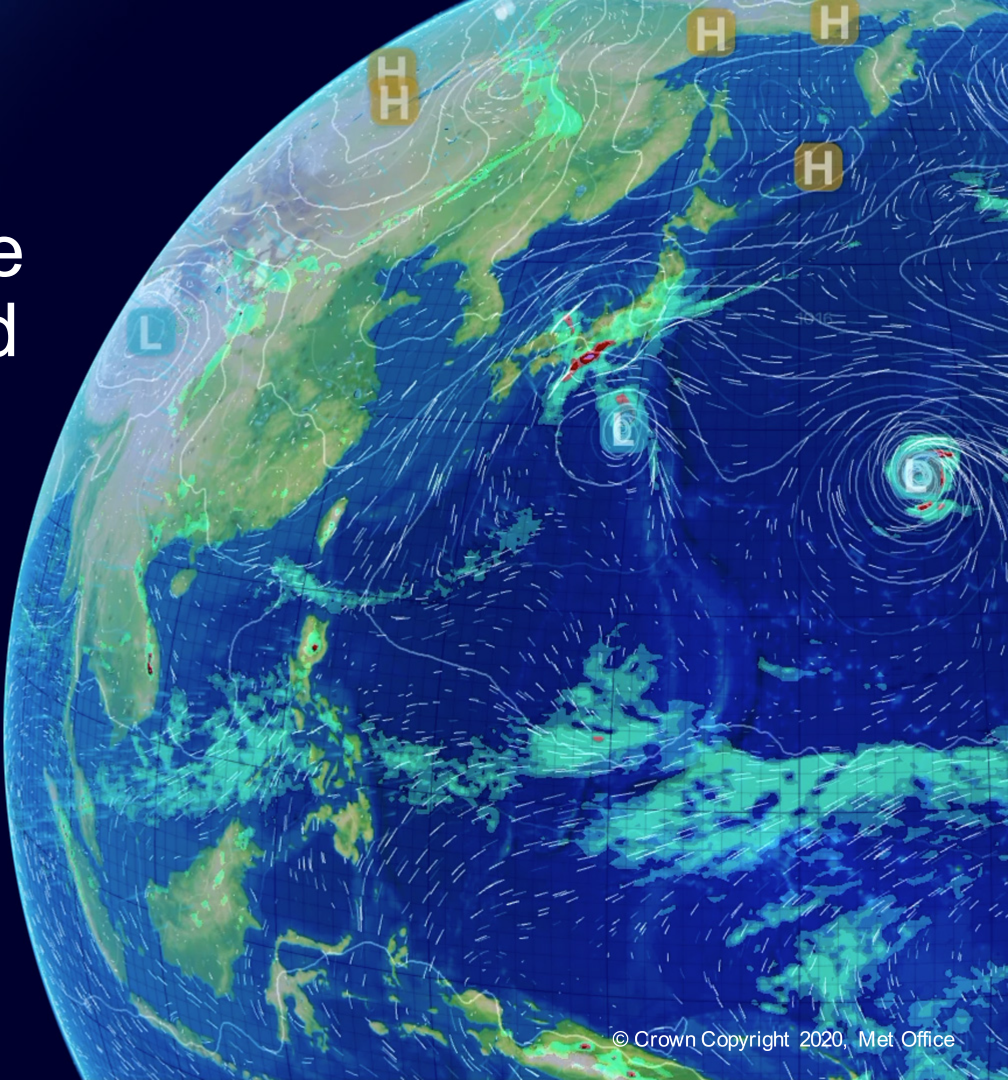
Use of uncertainty information from reference observations in model and satellite cal/val

Stuart Newman, Fabien Carminati, Heather Lawrence, Nils Wedi and Bill Bell

with thanks to contributions from Kirsti Salonen, Bruce Ingleby, Jacqueline Farnan, Stefano Migliorini, James Hocking and Niels Bormann

ECMWF/EUMETSAT NWP SAF Workshop on the treatment of random and systematic errors in satellite data assimilation for NWP

2 November 2020



Outline

- NWP as a satellite data validation tool (GAIA-CLIM study)
- Assessing NWP uncertainties with the GRUAN processor
- Uncertainties in surface emission
- Uncertainties due to spatial representativeness errors
- Uncertainties due to radiative transfer errors
- Summary

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 640276.

NWP as a tool for characterising Earth Observation data

GAIA-CLIM (Gap Analysis for Integrated Atmospheric ECV CLImate Monitoring) was an EU Horizon 2020 project undertaken to assess and develop our capability for the calibration/validation of long-term Earth Observation (EO) data sets using non-satellite reference measurements

Numerical weather prediction and reanalysis fields offer key advantages as a reference for assessing EO data quality

- Fields are spatially continuous
- Evolution is constrained by knowledge of physics/dynamics
- Atmospheric state analysis blends information from model and host of observations (satellite, sonde, surface, radio occulation, buoys, aircraft, …)

Question: to what extent is NWP a quantitative reference for assessing EO data sets and associated monitoring of ECVs?

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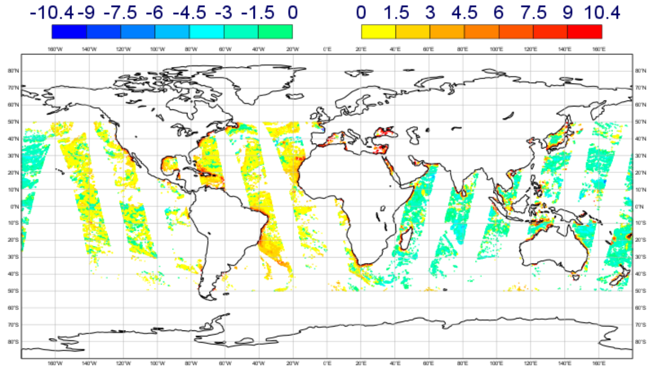
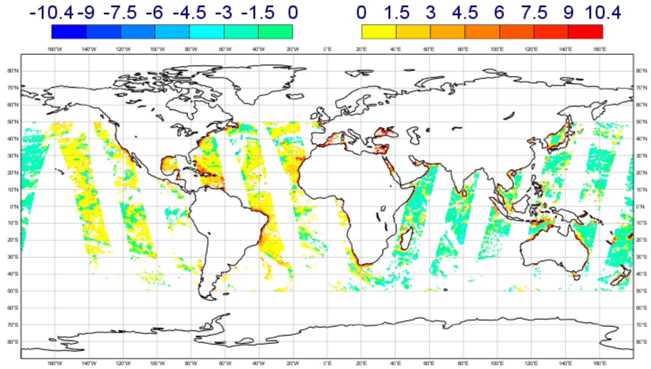
Assessing satellite data quality with NWP

Example: FY-3C MWRI 10.65 GHz H-pol channel

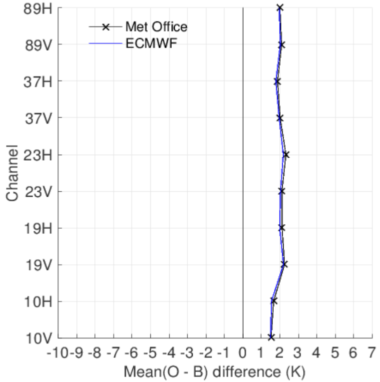
ECMWF O–B (minus global average)



Met Office O–B (minus global average)



Mean(O–B): Ascending – Descending



- Compare satellite observations with NWP fields (via radiative transfer model): **O-B**
- NWP outputs are of sufficient quality to diagnose satellite instrument biases (here calibration differs according to spacecraft position relative to the sun)

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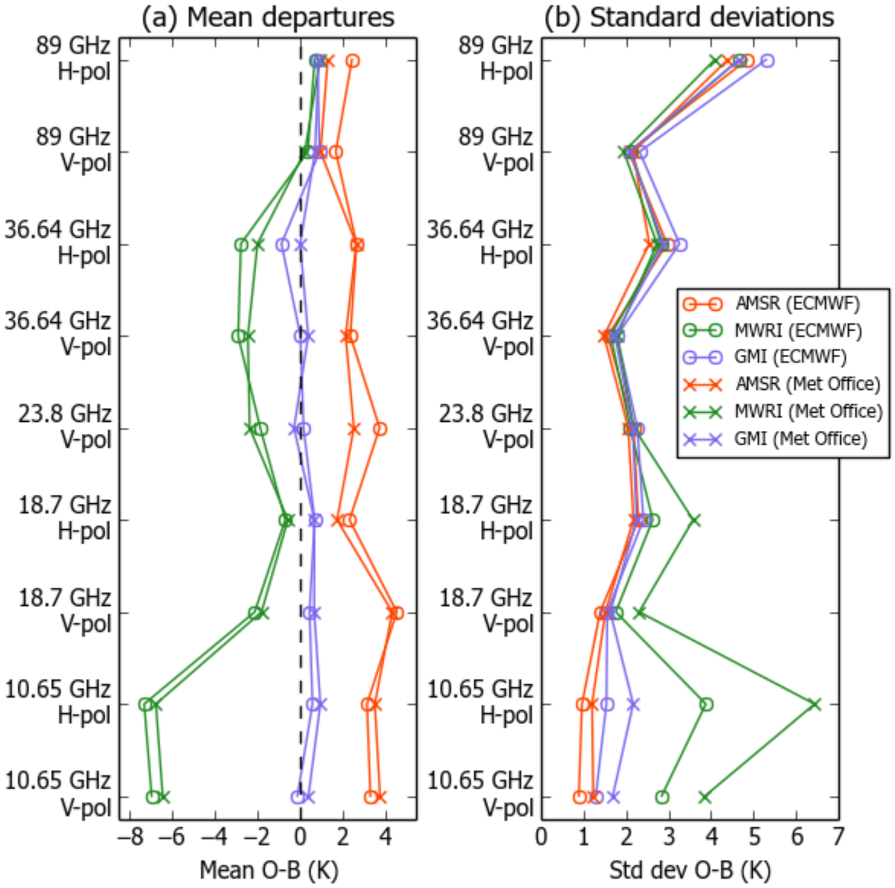
Satellite sensor intercomparisons

- ECMWF and the Met Office assessed O-B statistics for imagers AMSR2, MWRI and GMI
- Data were screened for cloud, analysed over sea only
- Find that GMI stands out with mean O-B departures within ±1 K
- But it is difficult to use NWP as an **absolute** reference due to uncertainties in surface emission



AMSR2 data during 2015; MWRI 2016; GMI 2016-17

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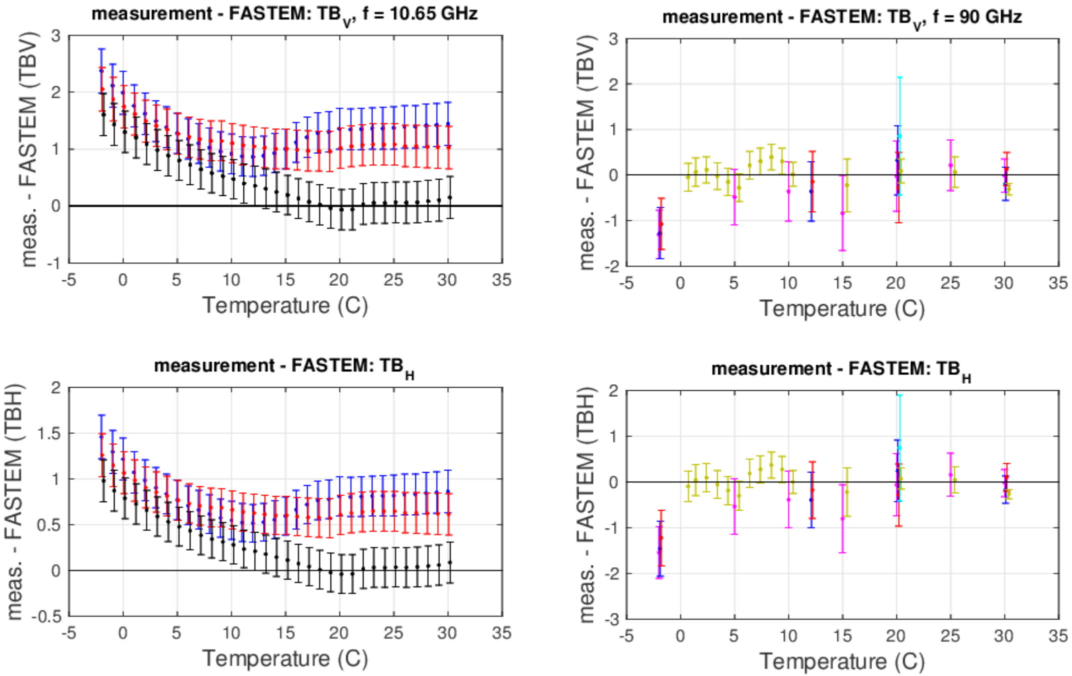
Comparing FASTEM to laboratory measurements with uncertainties

10.65 GHz | 90 GHz

V pol

H pol



Ellison 1996, S = 23.2°/oo
Ellison 1996, S = 30.255°/oo
Ellison 1996, S = 38.893°/oo

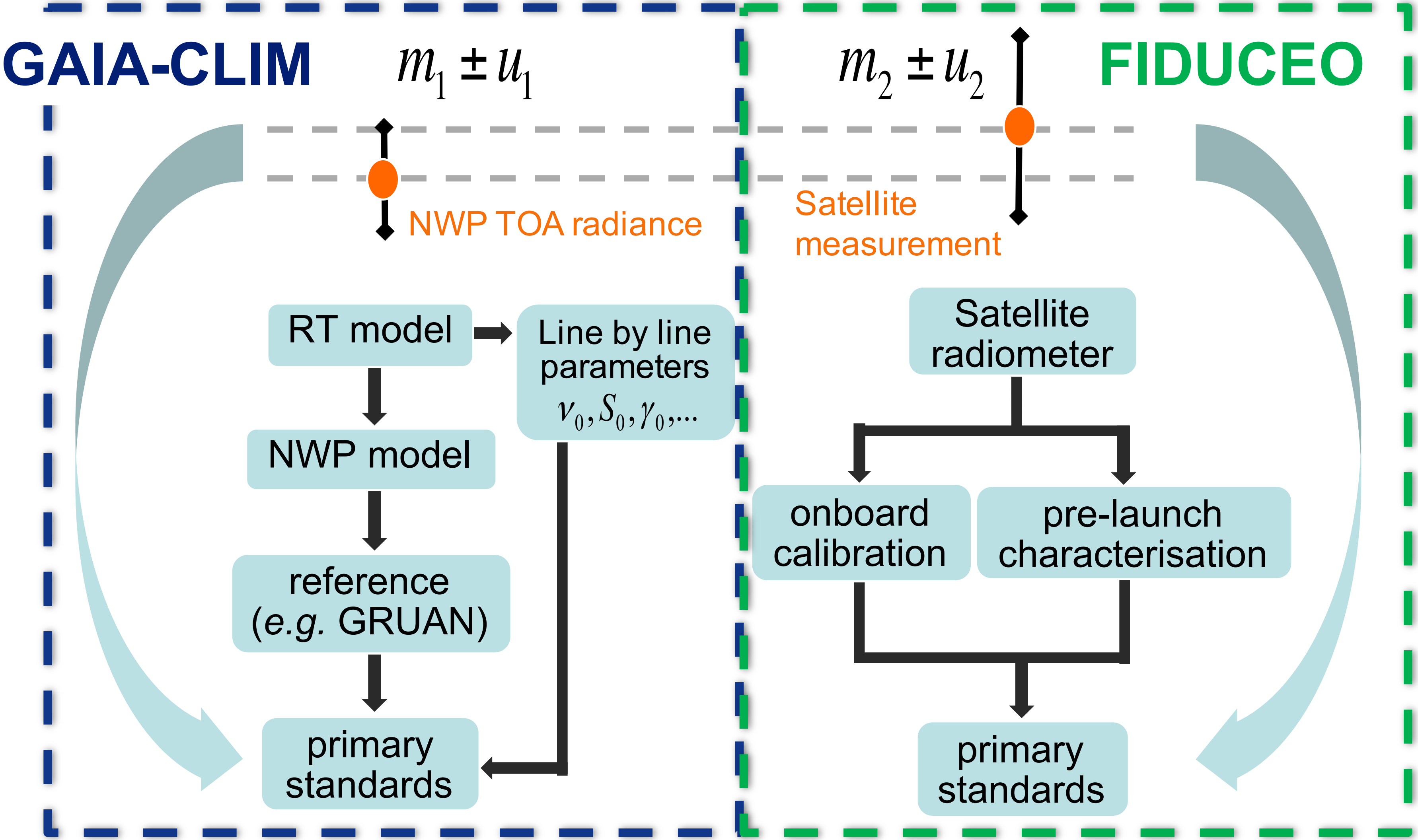
Seawater permittivity measurements

Ellison 2003, S = 35°/oo
Ellison 1996, S = 23.2°/oo
Ellison 1996, S = 30.255°/oo
Kaatze 1981 quasi data, S = 0°/oo
Richards 1991, S = 0°/oo

- Good agreement above 20 GHz
- Uncertainties ~ 0.5 – 1 K
- Disagreement exceeds measurement uncertainties at 5 – 20 GHz, low T
- But FASTEM in better agreement with GMI observations in NWP
- Lab measurements wrong or compensating biases?
- Perhaps uncertainties should increase for 5 – 20 GHz, low temperatures

See **Lawrence et al.**, Journal of Quantitative Spectroscopy & Radiative Transfer 243 (2020) 106813

International Space Science Institute team activity led by Steve English on a reference quality model for ocean surface emissivity and backscatter


GAIA-CLIM
$m_1 \pm u_1$
$m_2 \pm u_2$
FIDUCEO
NWP TOA radiance
Satellite measurement
RT model
Line by line parameters $\nu_0, S_0, \gamma_0, \ldots$
NWP model
reference (*e.g.* GRUAN)
primary standards
Satellite radiometer
onboard calibration
pre-launch characterisation
primary standards

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GRUAN processor

- The GRUAN processor is a co-location and radiance simulation tool based on the NWP SAF Radiance Simulator
- NWP data are ingested alongside radiosonde reports from the Global Climate Observing System (GCOS) Reference Upper-Air Network (GRUAN)
- GRUAN processing corrects radiosonde measurements for known systematic errors and provides uncertainty estimates for temperature, humidity, wind, pressure, and geopotential height
- The GRUAN processor allows us to quantify differences between NWP fields and reference radiosonde profiles in both profile and radiance space

GRUAN sonde profile
NWP model profile
→ Horizontal / vertical interpolation
→ RTTOV calculation for sensor/channel
→ GRUAN output
→ NWP output

Carminati et al., Atmos. Meas. Tech., 12, 83–106, 2019

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Uncertainty estimation for NWP-GRUAN match-ups

$$\mathbf{S}_{\delta y} = \mathbf{HRH}^T + \mathbf{HWBW}^T\mathbf{H}^T + \mathbf{HS}_{int}\mathbf{H}^T$$

$$|m_1 - m_2| < k\sqrt{u_1^2 + u_2^2}$$

δy	NWP-GRUAN difference
$\mathbf{R}$	GRUAN uncertainty matrix (uncertainty components at each profile level added in quadrature)
$\mathbf{H}$	RTTOV Jacobian matrix
$\mathbf{W}$	Interpolation matrix between vertical grids
$\mathbf{S}_{int}$	Covariance of interpolation uncertainty

m_1	measurement 1 (NWP)
m_2	measurement 2 (GRUAN)
u_1	uncertainty in m_1
u_2	uncertainty in m_2
k	Coverage factor (expect inequality to be met for approx. 95.5% of match-ups for k = 2)

Immler et al., Atmos. Meas. Technol. 2010, 3, 1217–1231

For satellite channel i with coverage factor 2:

$$|\delta \boldsymbol{y}_i| < 2\sqrt{diag(\boldsymbol{S}_{\delta y})_i}$$

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GRUAN match-ups for any sensor

- We can use the GRUAN processor to simulate NWP and GRUAN TOA brightness temperature for any satellite sensor/channel
- Magnitude of NWP-GRUAN differences in radiance space can be used to validate estimates of NWP uncertainties applicable to O-B
- Example for upcoming mission: MWS on MetOp-SG, Met Office Unified Model vs. GRUAN
- New results with GRUAN Vaisala RS41 product

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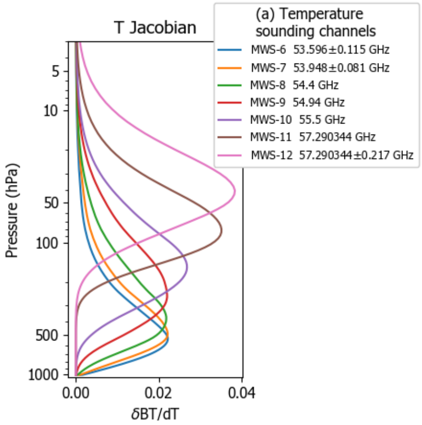
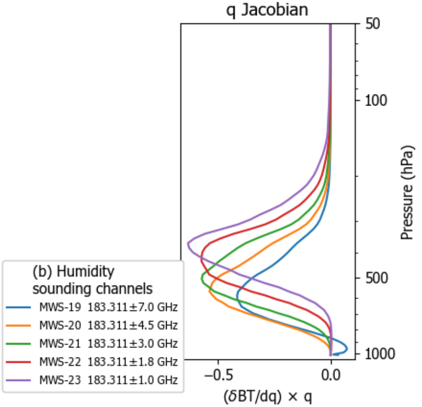
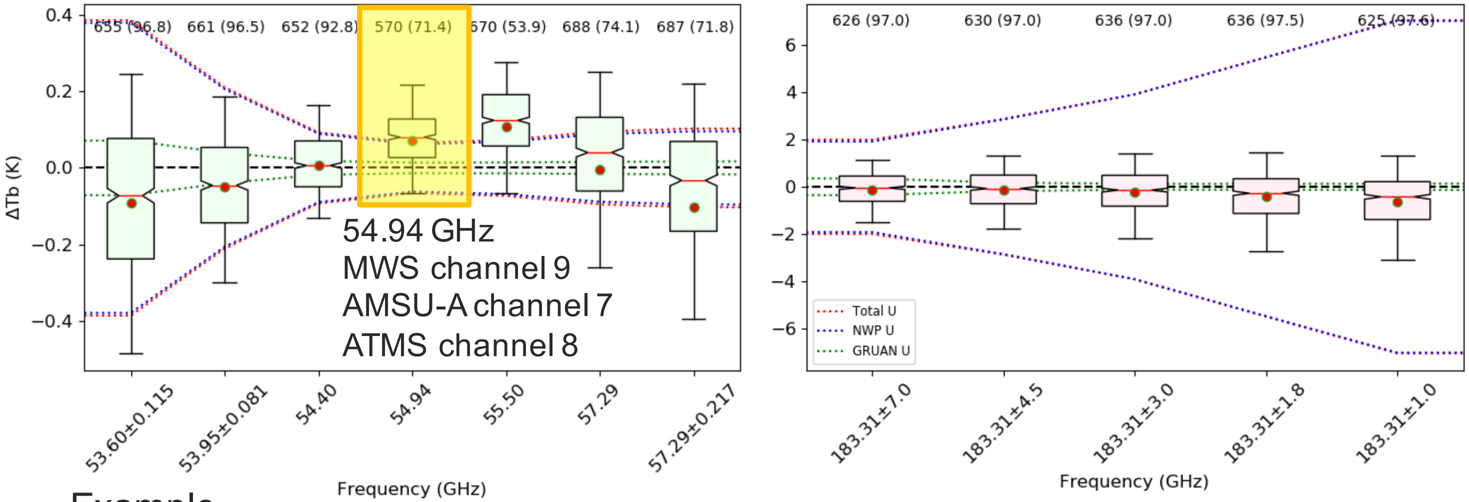
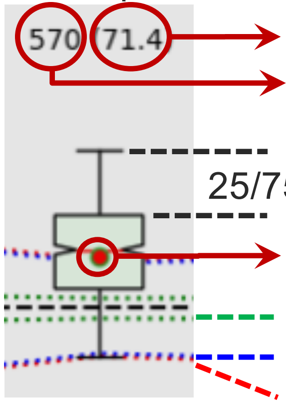




NWP$_{UM}$-GRUAN mid-northern-latitudes MWS



Example



71.4% of match-ups within k=2 uncertainty bounds

570 profile match-ups

25/75% and 5/95% bounds of NWP-GRUAN distribution

Mean NWP-GRUAN difference

Total estimated uncertainty GRUAN

Total estimated uncertainty NWP

Overall estimated uncertainty GRUAN + NWP

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GRUAN match-ups for MWS case study

How to explain finding fewer than 95% of match-ups within expected bounds?
Either there is a **systematic difference** NWP-GRUAN or uncertainties are **underestimated**

- We do not account for systematic NWP model biases in our uncertainty estimate (the **B** matrix only represents randomly distributed errors)
- We have used global mean **B** matrix uncertainties
- We neglect spatial representativeness errors
- The GRUAN uncertainty matrix **R** is sub-optimal
- Mean NWP-GRUAN differences are within ±0.1 K (estimated uncertainties up to 0.4 K) for temperature sounding channels; within ±0.7 K (estimated uncertainties ≥ 2 K) for humidity sounding channels
- Cf. MWS design requirement is for an absolute radiometric bias of less than 1 K for all channels

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Uncertainty for NWP ⇒ brightness temperature

$$u(T_B) = f(u(x_{NWP}), u(H), u(\Delta x), u(z,z'), u(cloud))$$

Uncertainties in NWP *T*, *q* mapped to brightness temperature

- ❑ Estimate from NWP-GRUAN

Uncertainties in RT modelling

- ❑ Line-by-line to fast model
- ❑ Spectroscopic uncertainty
- ❑ Surface emissivity

Uncertainties due to scale mismatch

- ❑ Observation scale ≠ model scale
- ❑ Natural scale << obs and model

Uncertainties due to vertical interpolation

- ❑ GRUAN processor

Uncertainties due to residual cloud after screening

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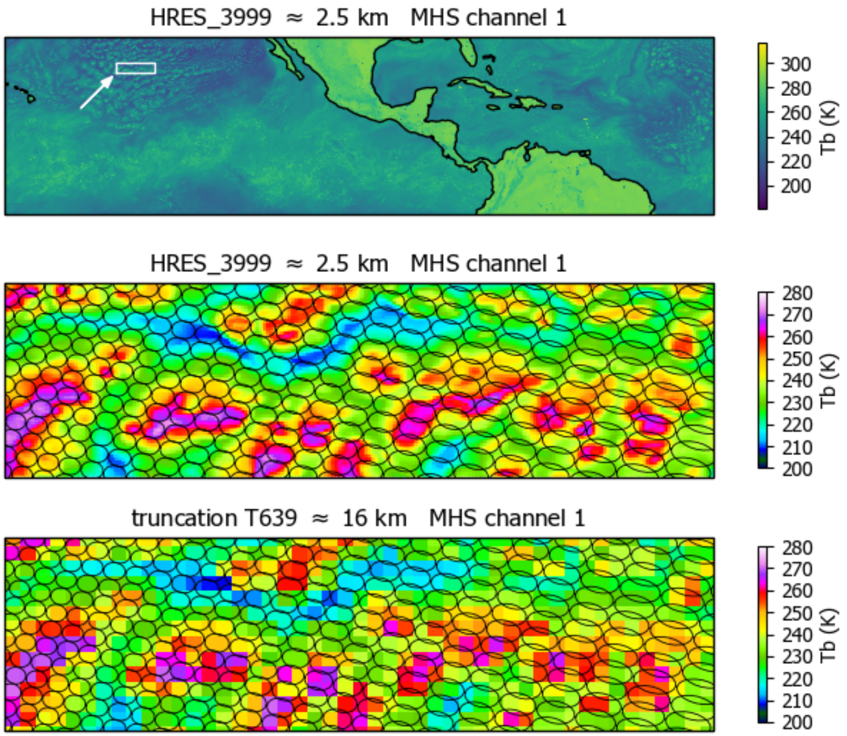
Uncertainties due to scale mismatch



- ECMWF cubic octahedral grid with resolution TCo3999, equivalent to a horizontal resolution of ~2.5 km – use as a proxy for realistic fine-scale structures
- Truncate field resolution to obtain fields at degraded spatial resolution
- Use NWP SAF Radiance Simulator (RTTOV-SCATT) to map fields into observation space for MHS channels 1-5
- Aggregate high-resolution simulations within satellite FOVs ➔ compare with model interpolation to FOV centre

Data from Nils Wedi

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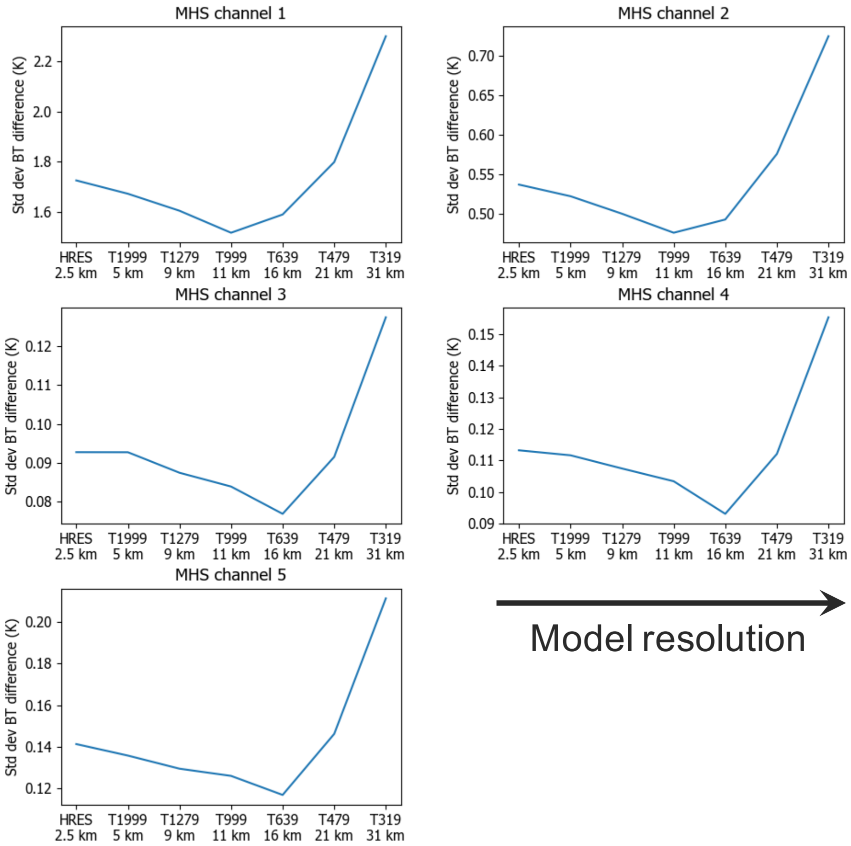
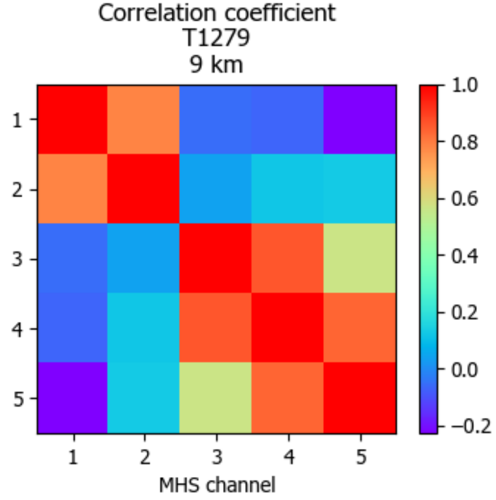
Spatial representativeness uncertainties



- Brightness temperature difference FOV-integrated high resolution data versus FOV-centre model interpolation at different resolutions
- Std dev of differences is approx. 0.1 K for MHS channels 3-5 at model resolution ~16 km

Std dev difference interpolation vs high resolution footprint



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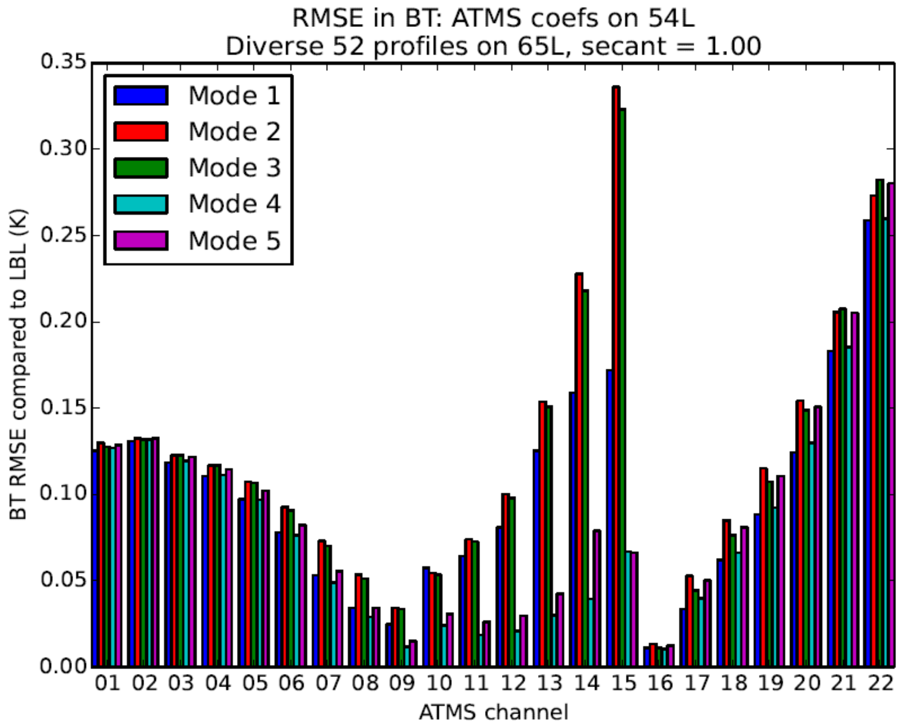
Uncertainties in radiative transfer modelling: line-by-line to fast model uncertainties



Temperature sounding channels

Water vapour

up to 0.3 K

- Comparing RTTOV and line-by-line brightness temperatures
- Errors are introduced due to optical depth regression and RTTOV interpolation between profile levels

James Hocking

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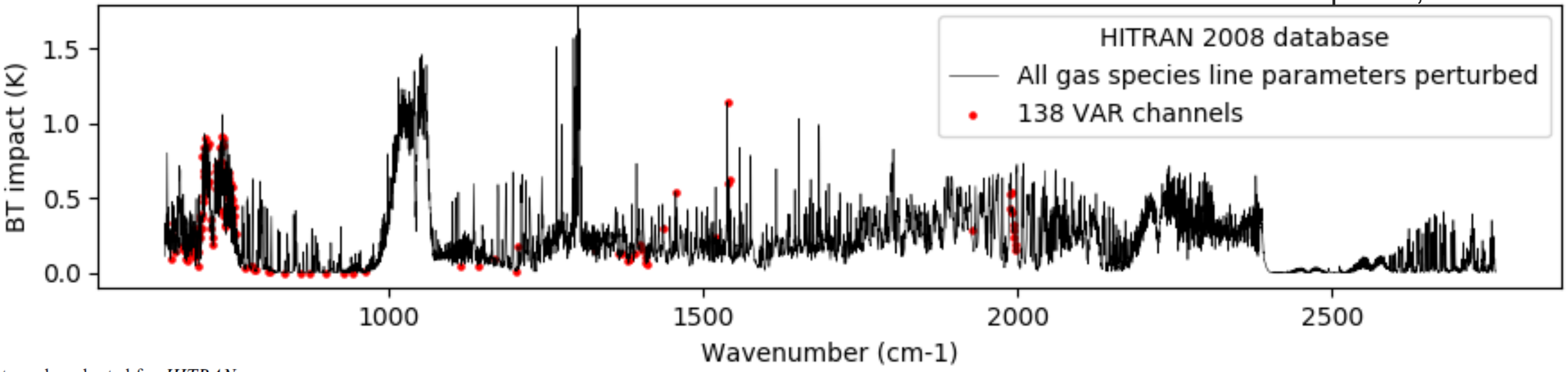
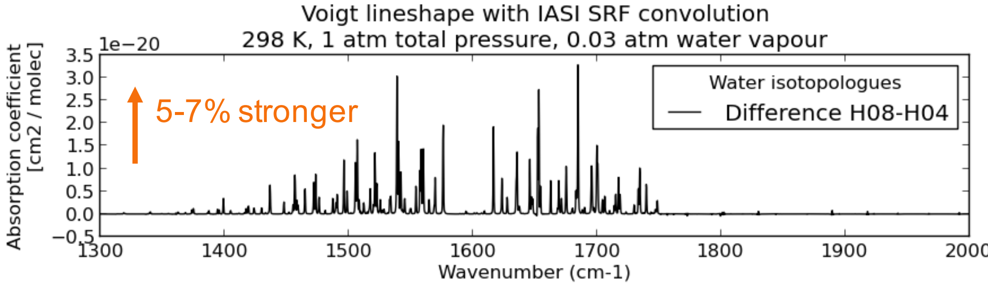
Uncertainties in radiative transfer modelling: spectroscopic uncertainties

Standard atmosphere, IASI SRF



Uncertainty codes adopted for *HITRAN*

Line position and Air pressure-induced line shift (cm^{-1})		Intensity, half-width (air- and self-) and temperature-dependence	
Code	Uncertainty range	Code	Uncertainty range
0	⩾1. or Unreported	0	Unreported or unavailable
1	⩾0.1 and <1.	1	Default or constant
2	⩾0.01 and <0.1	2	Average or estimate
3	⩾0.001 and <0.01	3	⩾20%
4	⩾0.0001 and <0.001	4	⩾10% and <20%
5	⩾0.00001 and <0.0001	5	⩾5% and <10%
6	<0.00001	6	⩾2% and <5%
		7	⩾1% and <2%
		8	<1%



Summary

- The NWP framework is shown to be useful in identifying (e.g. geographic) satellite biases
- Surface emission uncertainties are a limitation in the NWP validation of microwave imagers
- GRUAN processor is a first step towards establishing traceable uncertainty for NWP fields
- The uncertainty budget for NWP-GRUAN differences is incomplete, e.g. neglect of systematic model biases, sub-optimal GRUAN uncertainty matrix
- Spatial representativeness uncertainties can be estimated using high resolution fields as a proxy for fine-scale atmospheric structures (MHS example)
- Radiative transfer uncertainties: fast model errors can be constrained, uncertainties due to spectroscopy have likely inter-channel correlations

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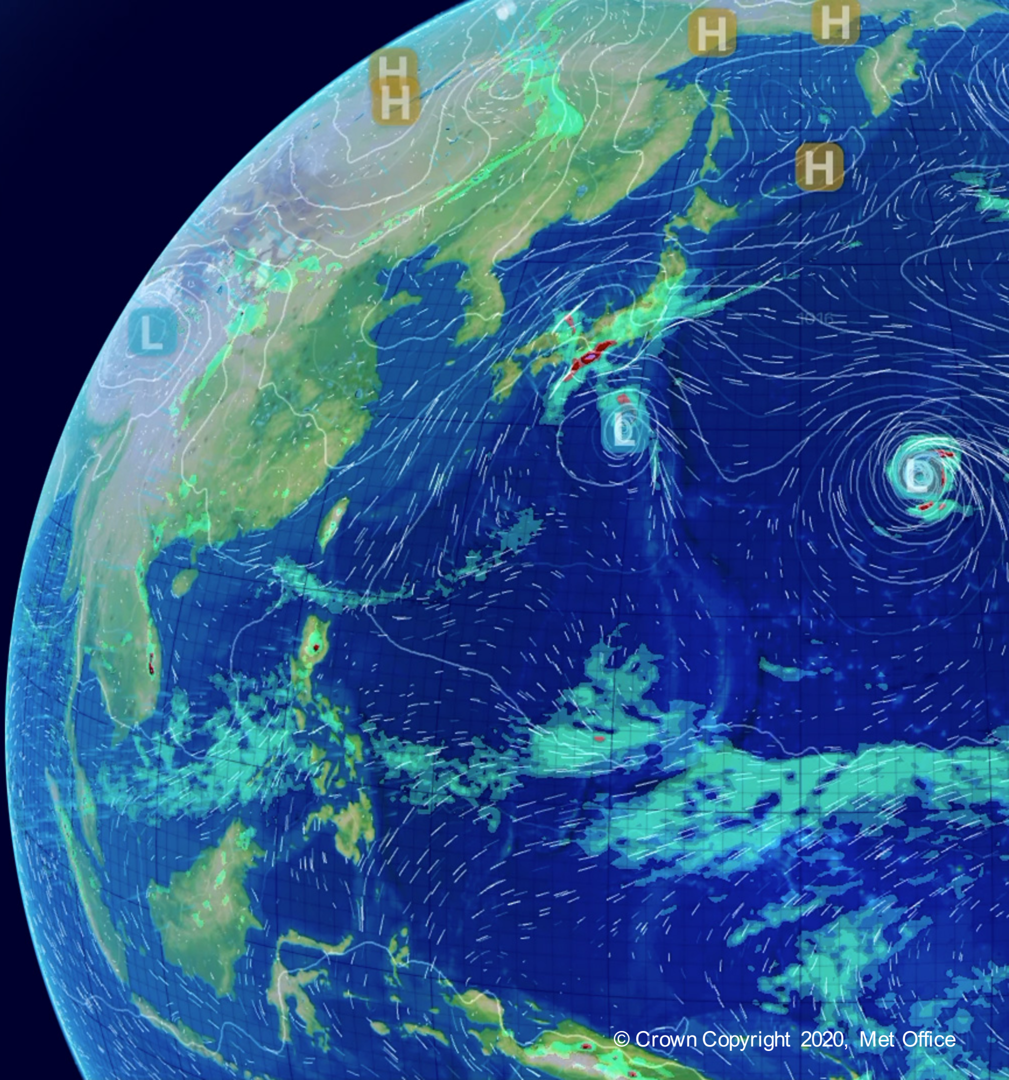
Thanks for your attention



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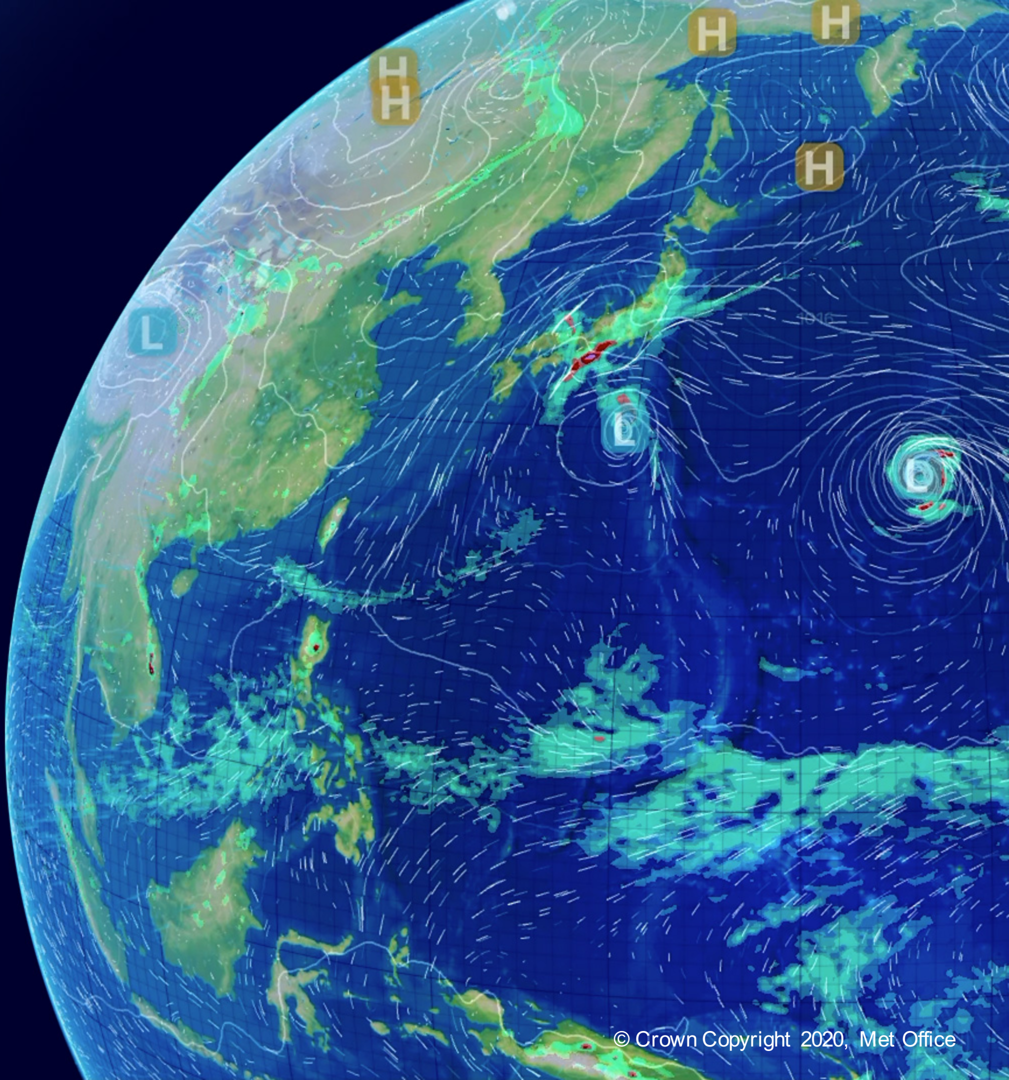
Supplementary slides



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GRUAN match-ups for MWS

Summary for different GRUAN sites (MWS channel 8)

GRUAN site	Match-ups within k=2 bounds	Estimated total uncertainty	NWP-GRUAN mean difference
Lindenberg, Germany (mid northern latitudes)	93%	0.09 K	0.00 K
Lauder, New Zealand (mid southern latitudes)	91%	0.09 K	0.01 K
Sodankylä, Finland (northern latitudes)	96%	0.15 K	0.05 K
Ross Island, Antarctica (southern latitudes)	97%	0.15 K	-0.02 K
Singapore (tropical)	56%	0.09 K	-0.16 K

- Met Office Unified Model vs. GRUAN 01/01/2020 to 30/06/2020
- Tropical site Singapore is an outlier compared to mid- and high-latitude sites

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The reduced Chi-square test gives the overall agreement, accounting for inter-channel correlation:

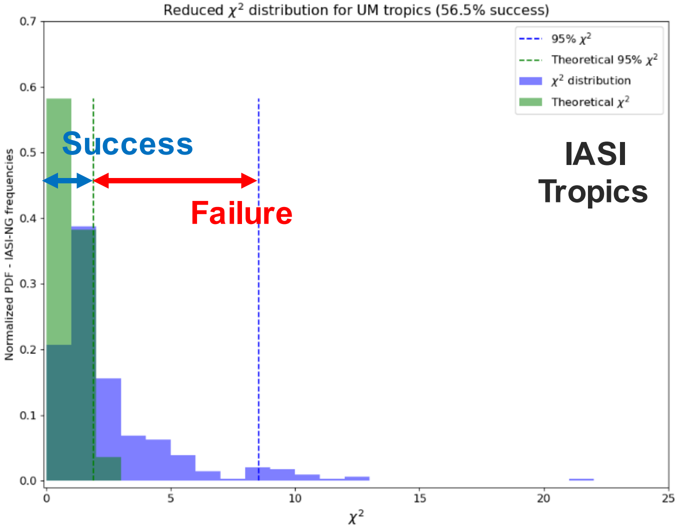
$$\tilde{X}^2 = \frac{1}{c}\left(\delta \boldsymbol{y}_i - \overline{\delta \boldsymbol{y}}\right)^T \boldsymbol{S}_{\delta y}^{-1}\left(\delta \boldsymbol{y}_i - \overline{\delta \boldsymbol{y}}\right)$$

where *c* is the number of degrees of freedom

$\tilde{X}^2_{calc}(95\%) > \tilde{X}^2_{theo}(95\%)$ means:

- One (or more) component of $\boldsymbol{S}_{\delta y}$ have been underestimated, and/or
- Missing unforeseen sources of uncertainty

	Polar NH	Mid NH	Tropics	Mid SH	Polar SH
IASI-NG	83.9%	88.4%	56.5%	78.2%	91.5%
MWS	83.3%	89.4%	62.2%	81.3%	95.5%



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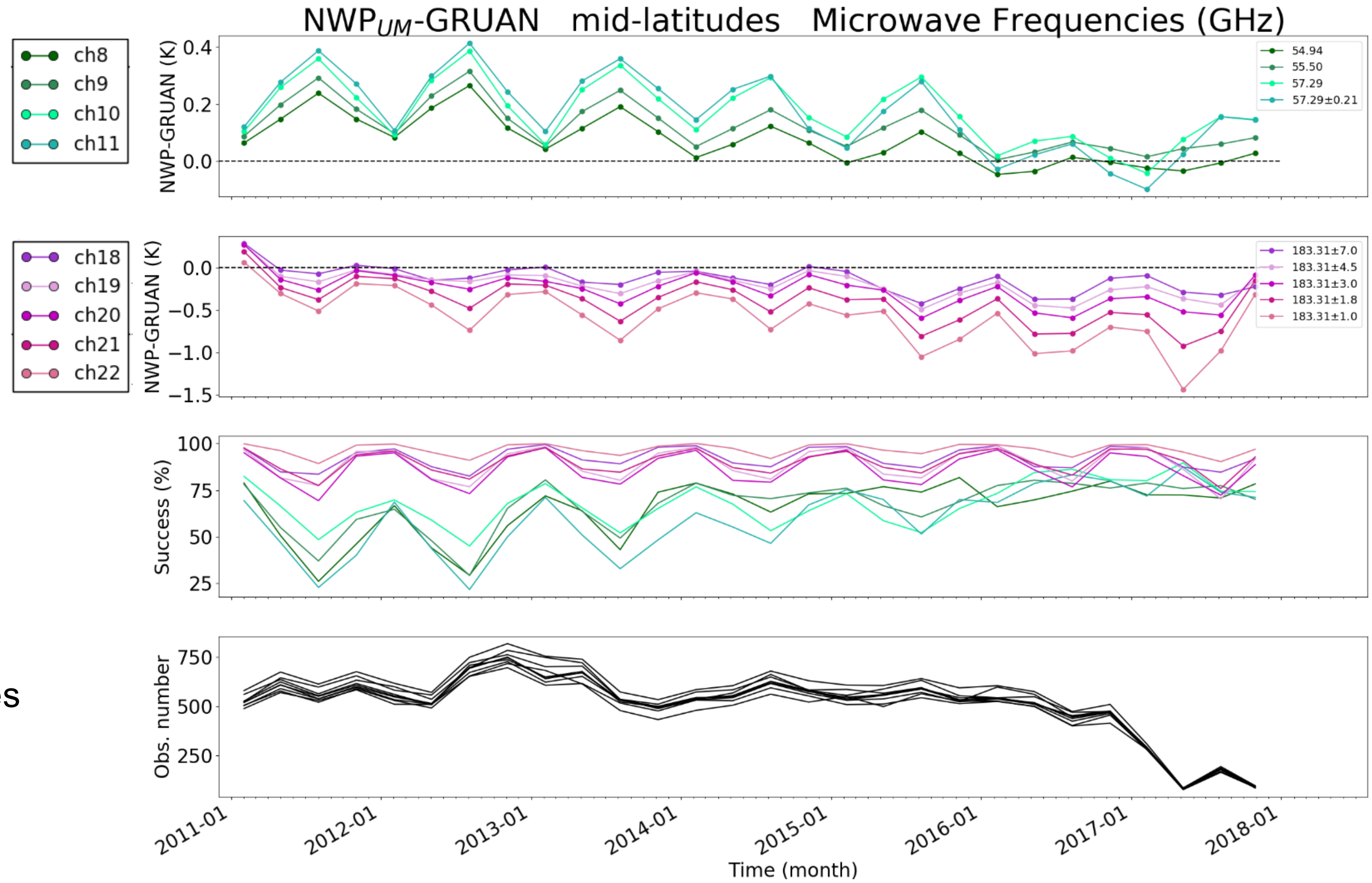
ATMS temperature sounding channels

ATMS humidity sounding channels

GRUAN RS92 sondes



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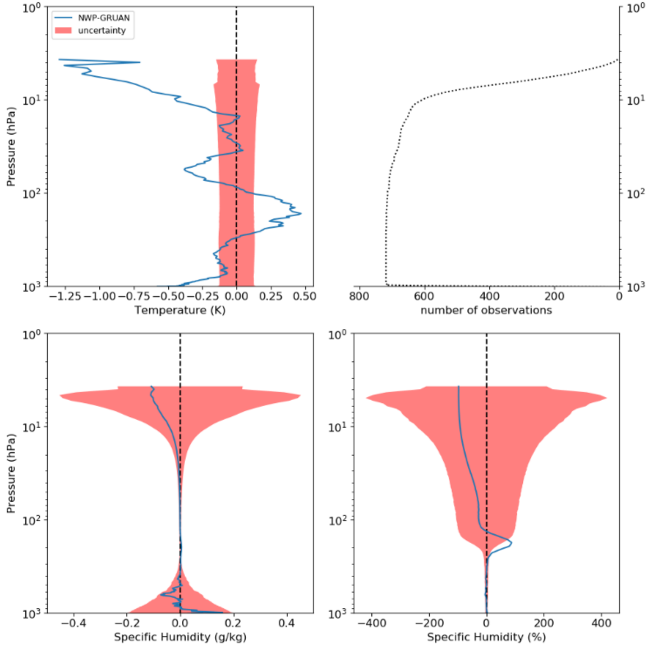
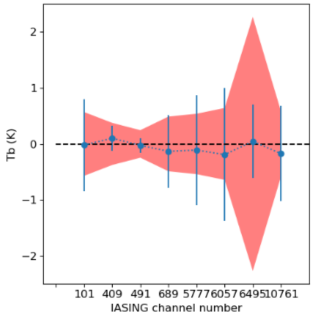
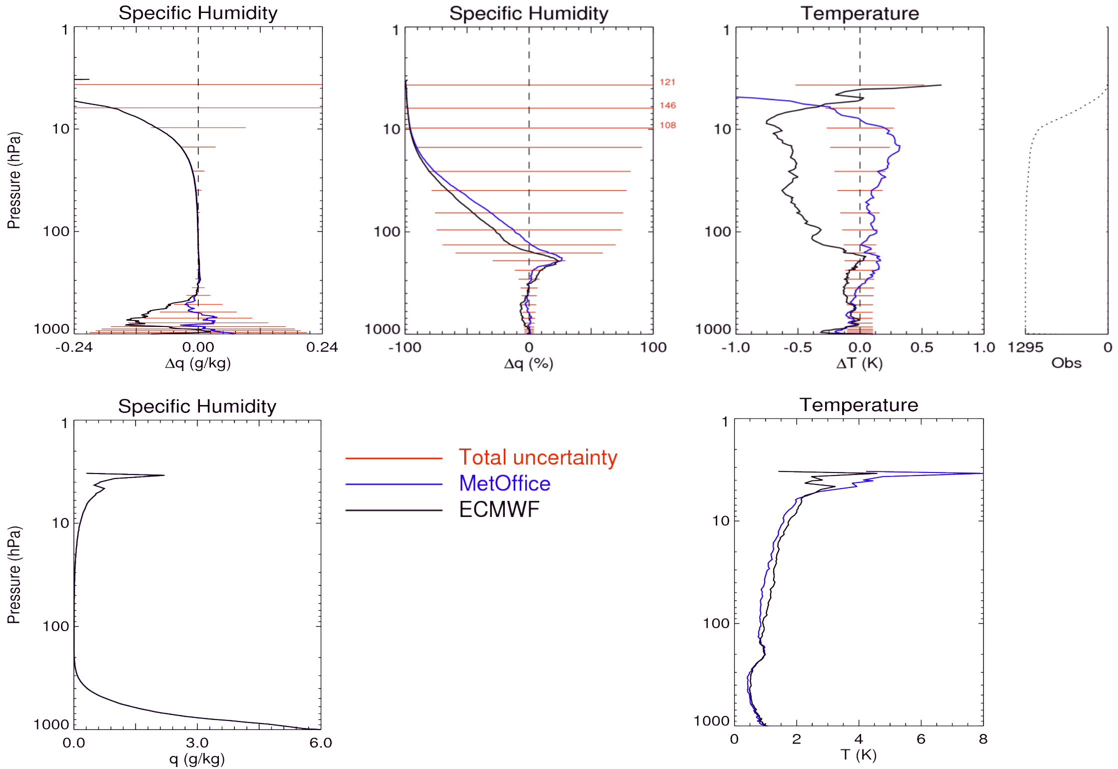
NWP – GRUAN: Lindenberg, 2013





NWP – GRUAN: Lindenberg, 2020



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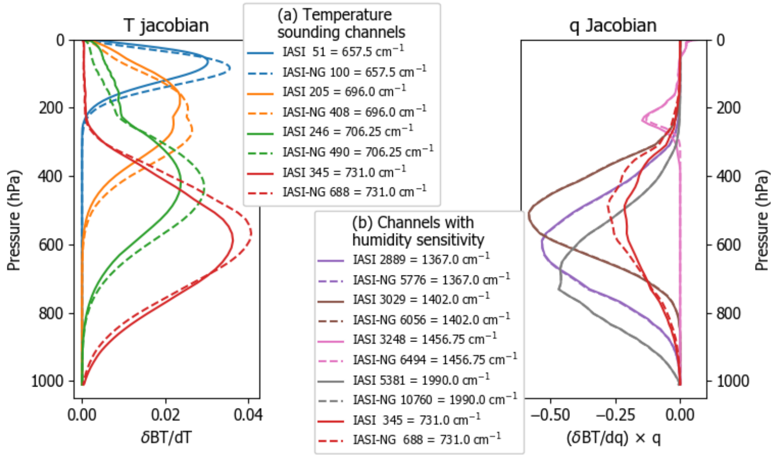
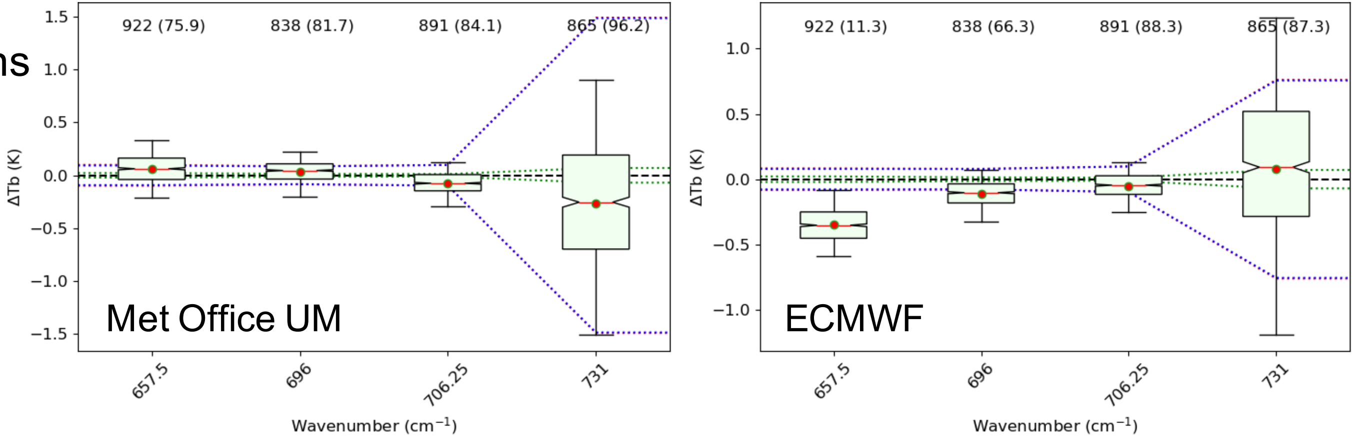
GRUAN match-ups for IASI-NG



One way to reconcile the spread of NWP-GRUAN distribution with NWP+GRUAN uncertainty estimates is to inflate the total uncertainty to achieve 95.5% within k=2 bounds

IASI-NG channel at 706.25 cm^{-1}: comparisons meet 95.5% threshold if total uncertainty is increased from 0.10 K (both centres) to 0.13 K (ECMWF), 0.15 K (Met Office)



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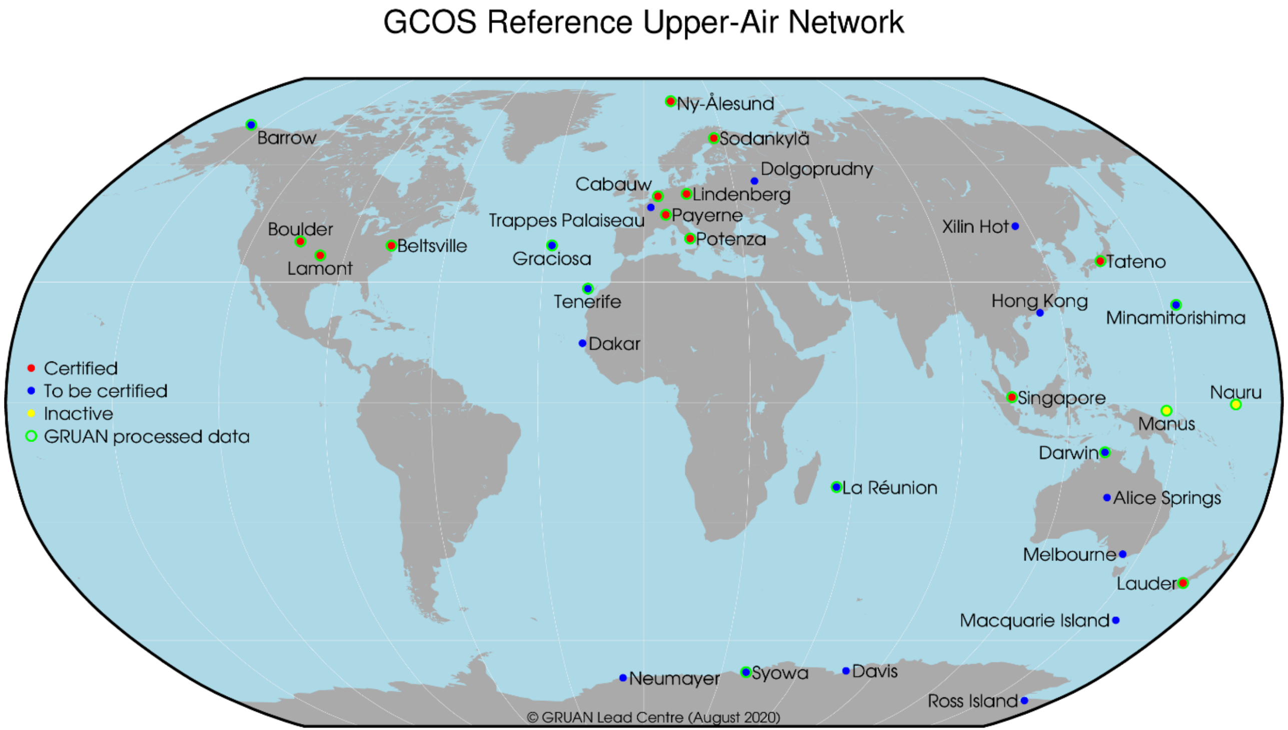

GRUAN has 32 sites (2 inactive)

- Measurements are traceable to a SI unit or an internationally accepted standard
- Data processing corrects for all known errors and biases
- Provides best estimate of the vertically resolved measurement uncertainty

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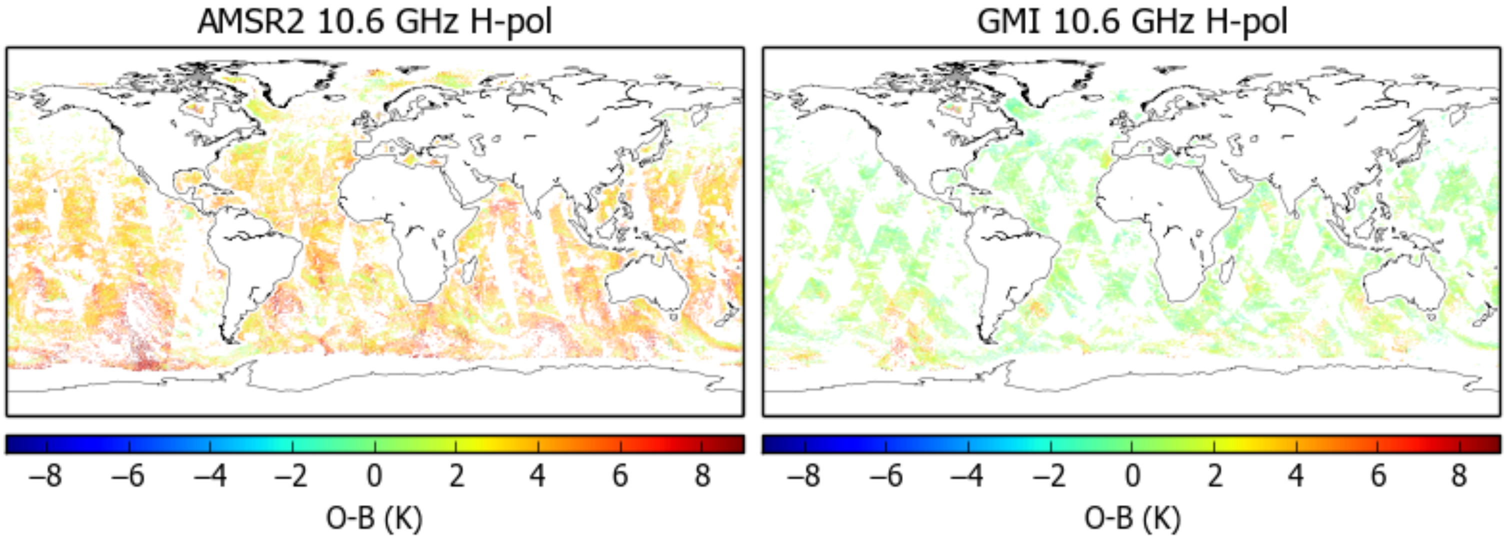

O-B maps for AMSR2 and GMI show systematic differences between sensors

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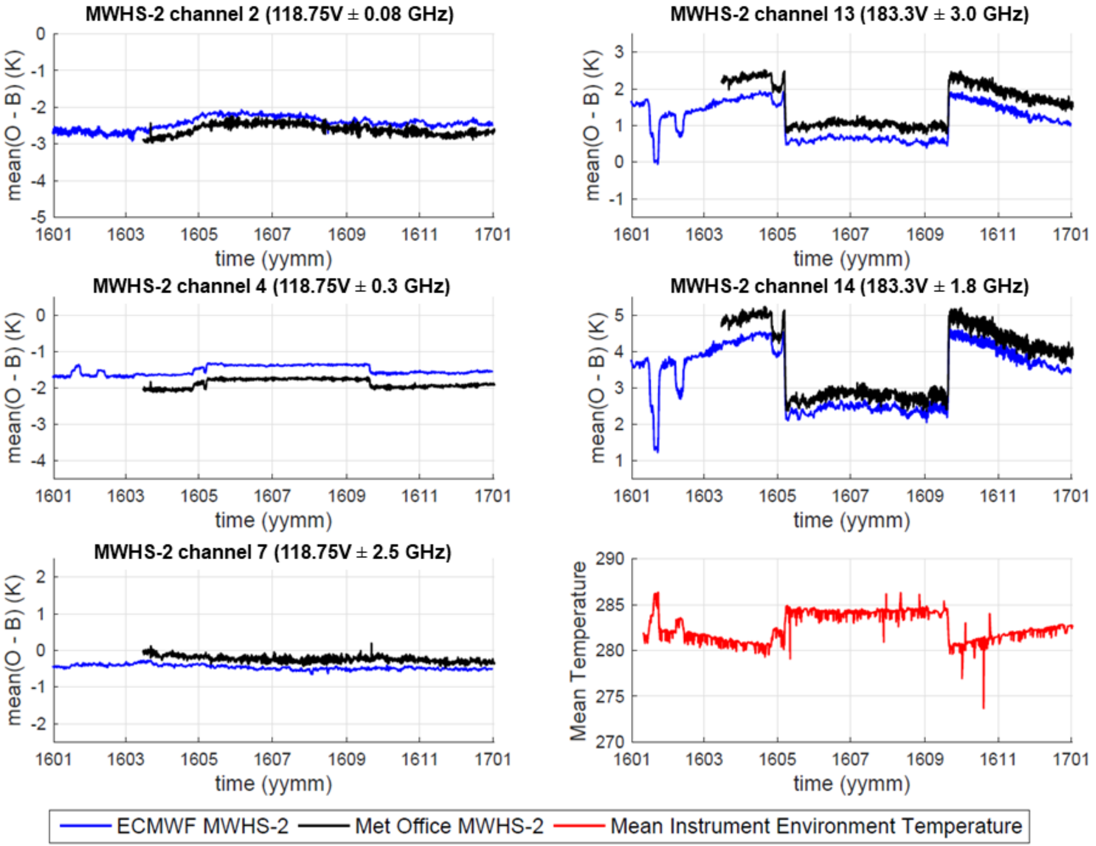
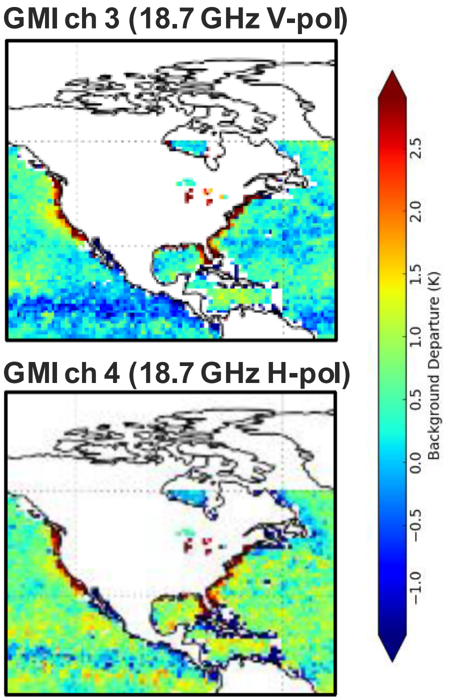
NWP O-B studies can detect time-varying biases (MWHS-2) and RFI (GMI)





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