Research collaborators for large ensemble simulations

Empirical optimal vertical localization derived from large ensembles

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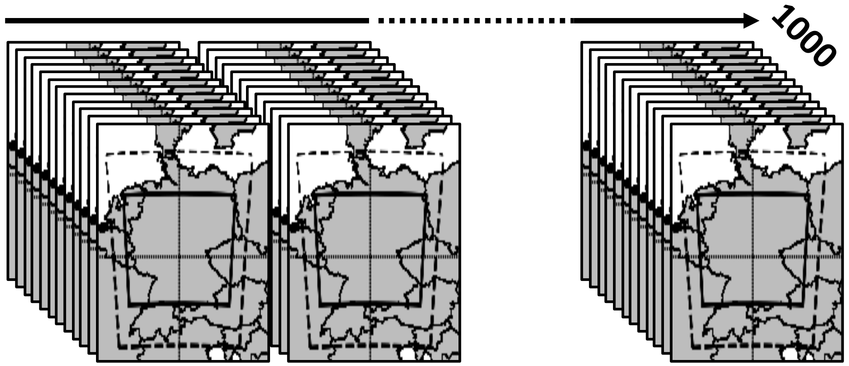
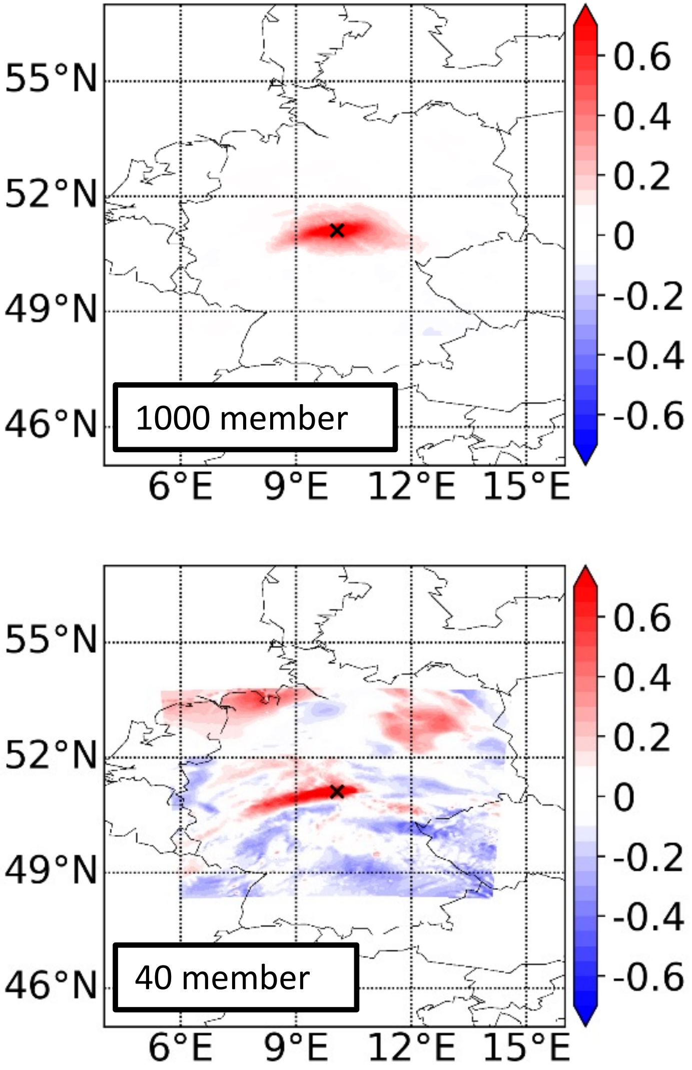
Outline

1. Empirical Optimal Localization (EOL) method
2. Results
   a. Optimal model space covariance localization
   b. Optimal gain localization for satellite observations
3. Take-home messages



Motivation



Example for spurious correlations on convective scales (Correlation of T2m to T2m)

Data assimilation heavily relies on accurate error covariance estimates

$$K = P^b H^T \left(H P^b H^T + R \right)^{-1}$$

Spread and weight observation information

Sampling errors in error correlations pose severe issue for data assimilation requiring localization

$$cov(\Delta x^b, \Delta y^b) = r(\Delta x^b, \Delta y^b)\, \sigma(\Delta x^b)\, \sigma(\Delta y^b)$$

Different reasons why we need localization?

1. **Sampling errors**
   (e.g., spurious correlations)
2. **Rank deficiency**
   (e.g., regularization / matrix inversions)
3. **Algorithm efficiency**
   (e.g., degrees of freedom in LETKF)

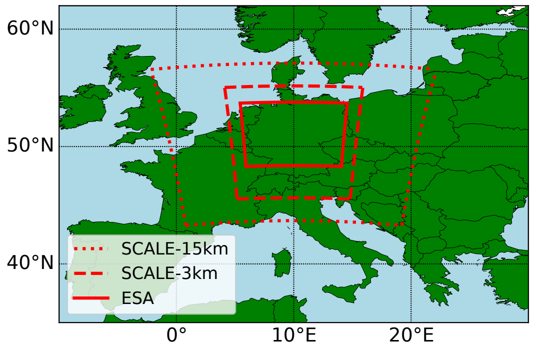
Motivation: Better understanding of error covariances and localization

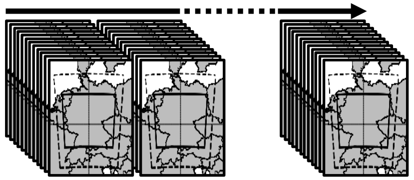
Our approach for fundamental research:

- Apply large ensemble to study sampling errors and improve localization
- 1000-member ensemble **(Necker et al. 2020)** provides background ensemble forecasts over Germany with 3km horizontal resolution and 30 vertical levels

Experimental setting:

- We assume 1000-member correlation as truth (r^{1000})
- Subsampling strategy: 25 40-member subsample correlations (r^{40})
- First guess: 3h lead time background convective-scale forecasts





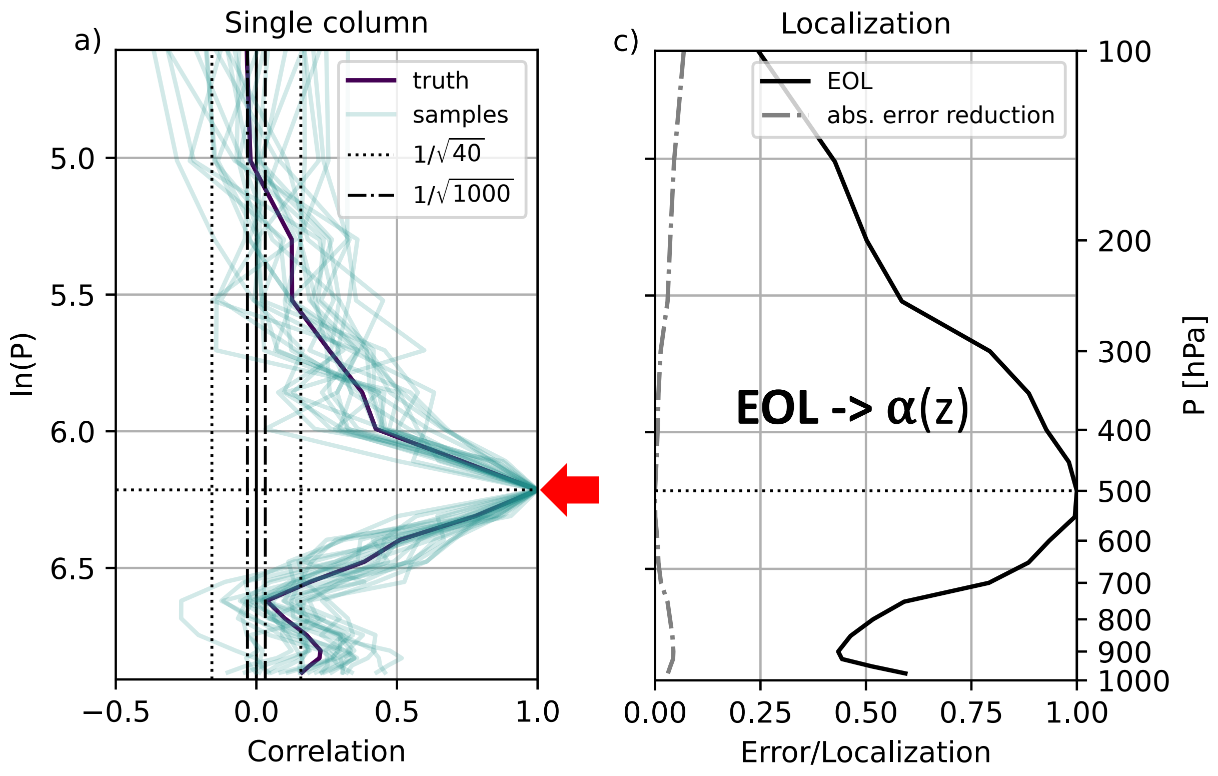
Main research questions:

a) How can we improve state-of-the-art vertical localization approaches?

b) How to achieve positive-definiteness of derived covariance and localization matrices?

c) How should we localize vertical error correlations of non-local visible and infrared satellite observations?

Empirical Optimal Localization (EOL) – Example for single vertical column



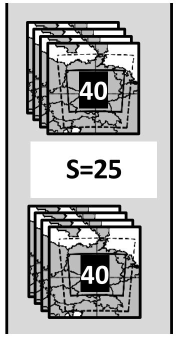
Goal: Derive an optimal localization from 1000-member ensemble using subsampling strategy

Strategy: Minimize the MSD between sample correlations and the 1000-m correlation truth using cost function J

$$J(\alpha) = \sqrt{\sum_{s=1}^{S} \left(\alpha r_s^{40} - r^{1000}\right)^2}$$

Solving for α yields simple formula for optimal localization:

$$\rightarrow \quad \boxed{\alpha_{single} = \frac{\sum_{s=1}^{S} r_s^{40} r^{1000}}{\sum_{s=1}^{S} (r_s^{40})^2}}$$



α : Optimal localization factor

r^{40} : 40-member ensemble correlations

r^{1000} : 1000-member ensemble correlation

S : Number of 40-member subsamples

Single column example:

- Temperature to temperature sample correlations
- Reference level 500hPa to all other vertical levels

How does the Empirical Optimal Localization (EOL) method work?

Properties of the empirical optimal localization (EOL) method (see Necker et al. 2023)

- Requires large ensemble as truth
- Subsampling allows deriving optimal localization
- Optimizes the covariance (not necessarily the analysis)
- Approach can easily be adapted to estimate optimal localization directly for Kalman gain K

EOL can be computed for single correlations or correlations grouped in batches of interest:

Option 1:

$$\alpha_{single} = \frac{\sum_{s=1}^{S} r_s^{40} r^{1000}}{\sum_{s=1}^{S} (r_s^{40})^2}$$

Optimal localization for single correlations

- Ideal to study situation-dependence or variability

Option 2:

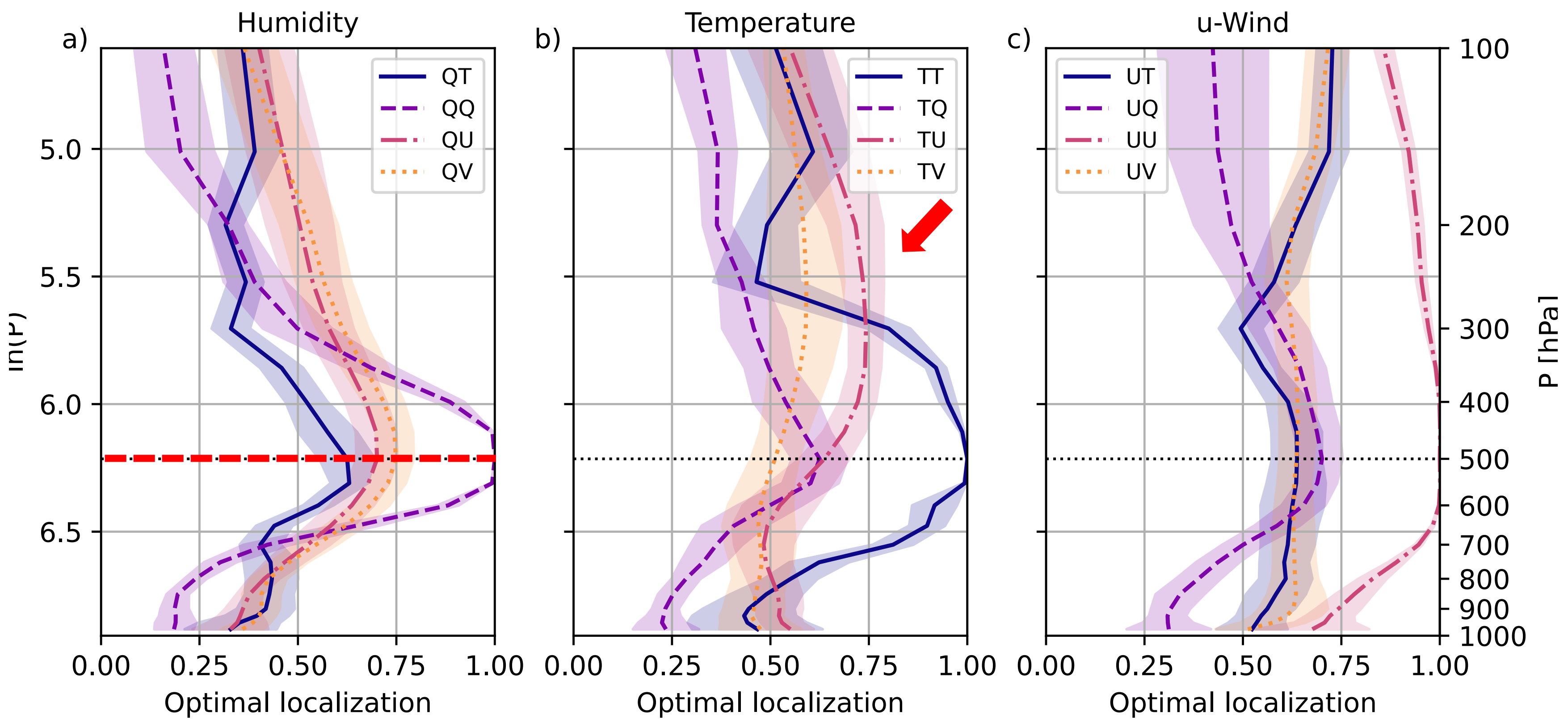
$$\alpha_{batch} = \frac{\sum_{s=1}^{S} \sum_{k=1}^{K} r_{s,k}^{40} r_k^{1000}}{\sum_{s=1}^{S} \sum_{k=1}^{K} (r_{s,k}^{40})^2}$$

Optimal localization for grouped correlations in batches defined by specific criteria

- Allows deriving: Domain-uniform, variable-, observation- or situation-dependent localization
- K: Number of combined correlations (e.g., variables, temproally, vertically, horizontally, …)

How should an optimal domain-uniform vertical localization look like?

T: Temperature / Q: Spec. humidity / U: Zonal wind / V: Meridional wind



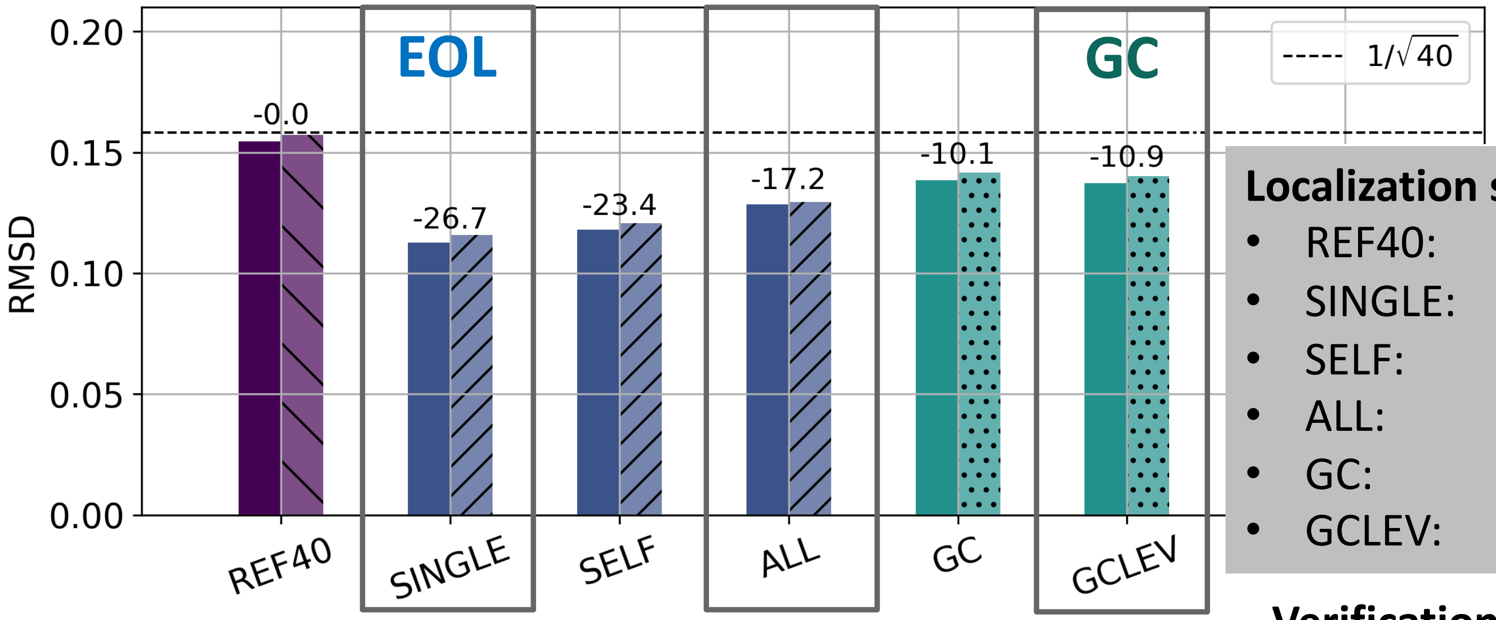
EOL for 500hPa

- Single variable pairs
- **Domain-uniform / non-adaptive**
- Shading: day-to-day variability
- **Reference level 500hPa**

Conclusions

- Substantially different localization scales and shapes for humidity, temperature, and wind
- Self- & cross-correlations behave systematically different
- Maximum of localization function not necessarily at reference level

Estimated error reduction (%) for different localization approaches



Configuration: Domain-uniform localization verified for two independent forecasts

Localization settings

- REF40: Reference without localization
- SINGLE: Variable-dependent EOL
- SELF: Self/cross correlation-dependent EOL
- ALL: One EOL function for all situations
- GC: Optimally tuned Gaspari-Cohn (GC)
- GCLEV: Height-dependent optimally tuned GC

Verification: Against 1000-member correlation truth

Conclusions

- GC vs ALL: Localization functions (shapes) can be improved compared to GC
- GC vs SINGLE: Variable or correlation dependent EOL outperform common methods by factor two

→ Applying better localization functions and treating variable pairs differently bears substantial room for improvements

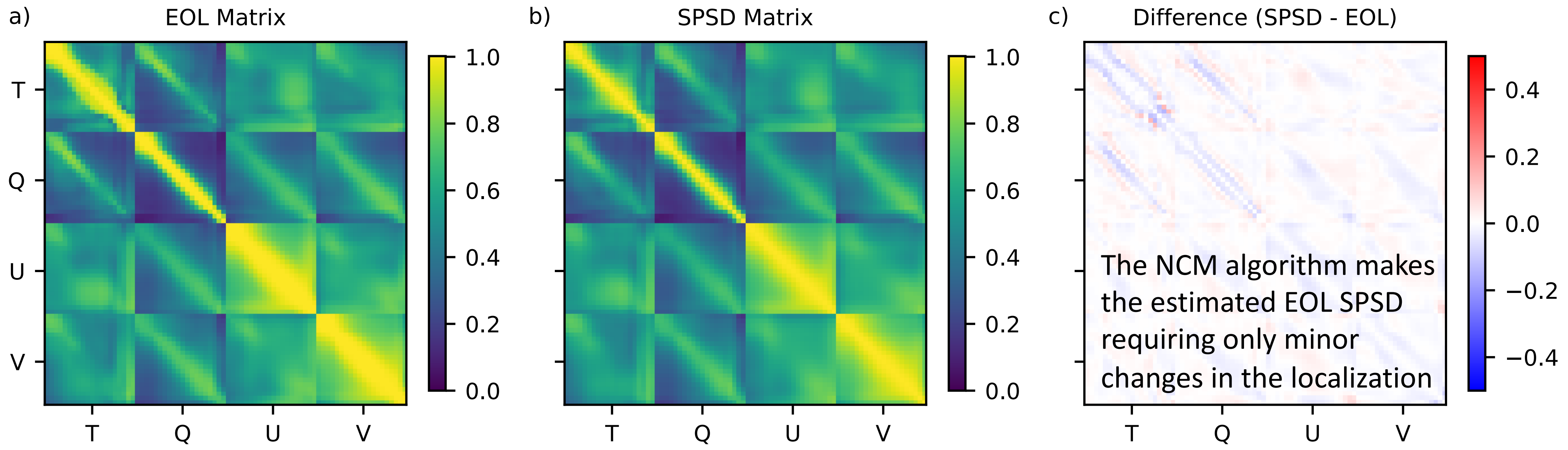
Does the EOL yield a symmetric positive semi-definite (SPSD) localization?

Localized cov-matrix: Needs to be symmetric positive semi-definite (PSD) to ensure a unique optimal analysis

Problem: Localization methods do not necessarily yield a positive semi-definite covariance matrix

<u>We tested different methods for achieving PSD of localization:</u>

1. **Fitting suitable localization functions such as GC:** GC ensures PSD by function design
2. **Regularization** or **eigen-decomposition:** Requires matrix manipulation to mitigate inflation of variances
3. **Nearest Correlation Matrix (NCM) algorithm** (Higham 2002): great results -> Potentially many use-cases in DA/ML



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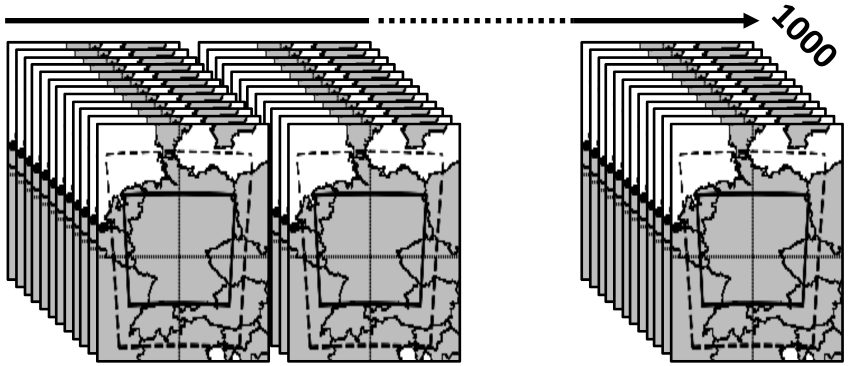
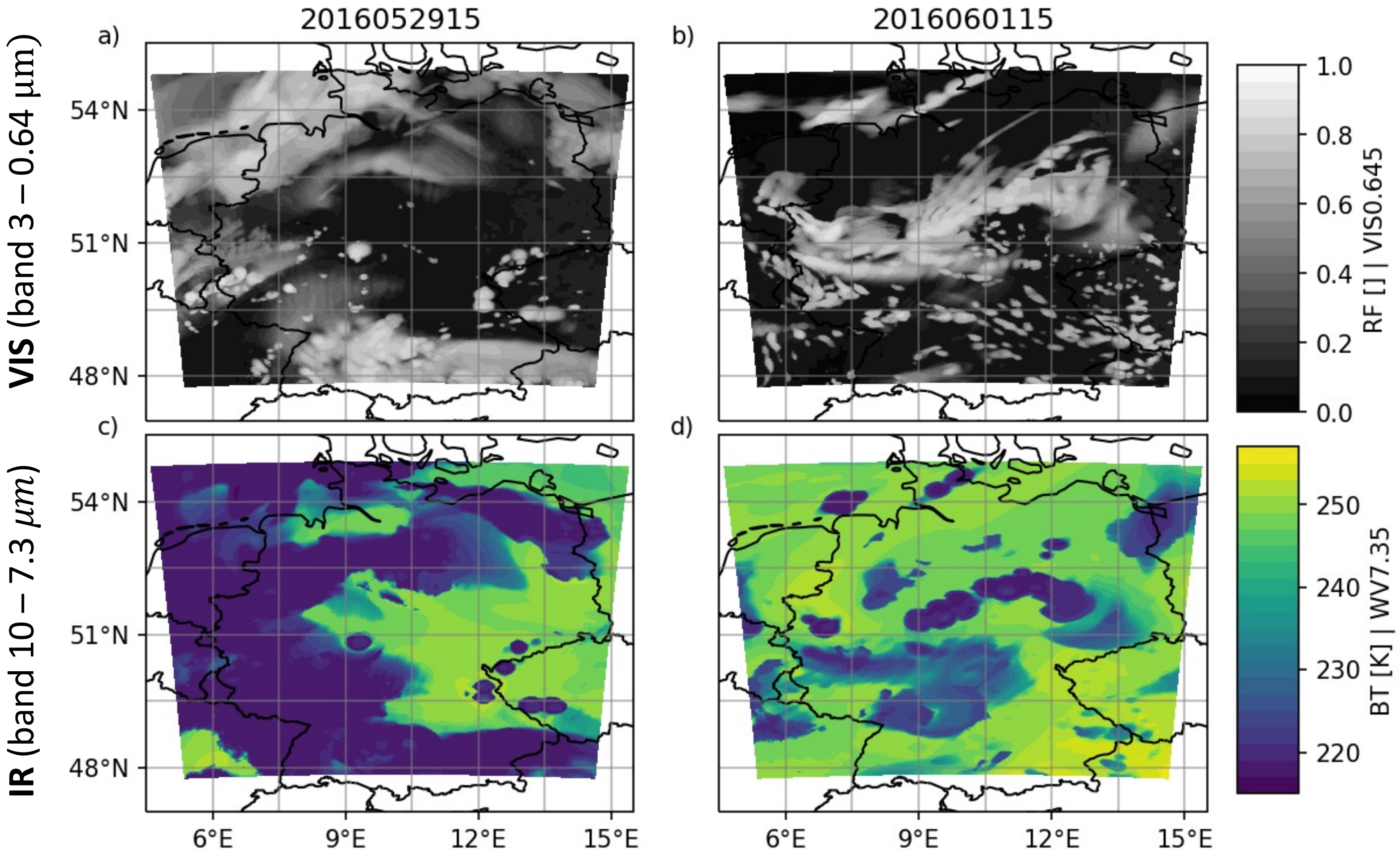


1000-member ensemble: Synthetic satellite images based on RTTOV



Setup:

- 2-days in May/June 2016, 15UTC
- 1000-member correlation as truth: r^{1000}
- Localization for 40-member ensemble assuming EAKF or LETKF DA

Today: Two channels of Himawari-8

- **IR** (band 10 – 7.35 μm)
- **VIS** (band 3 – 0.64 μm)

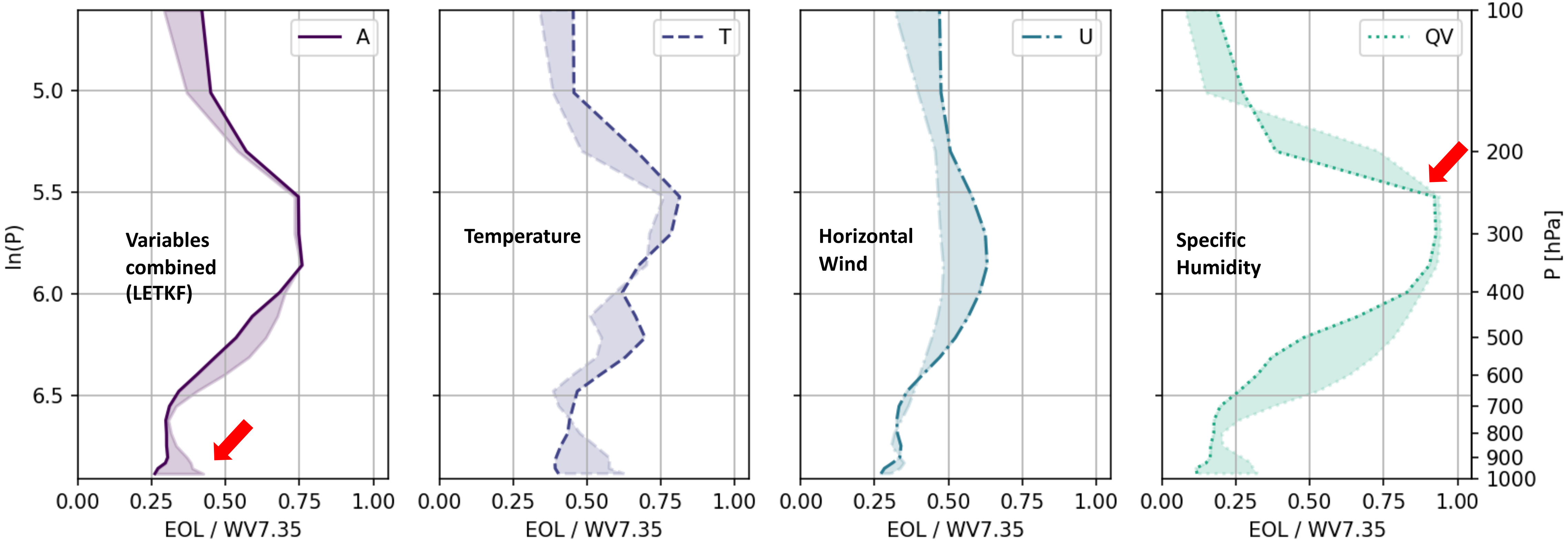
$$\Delta x = \alpha \, r \, \Delta y$$

Goal: *Localization α of error correlation r from satellite model equivalent y to state variable x*

Thanks to T. Honda for computing the synthetic satellite images

Domain-uniform EOL / Infrared 7.35µm channel

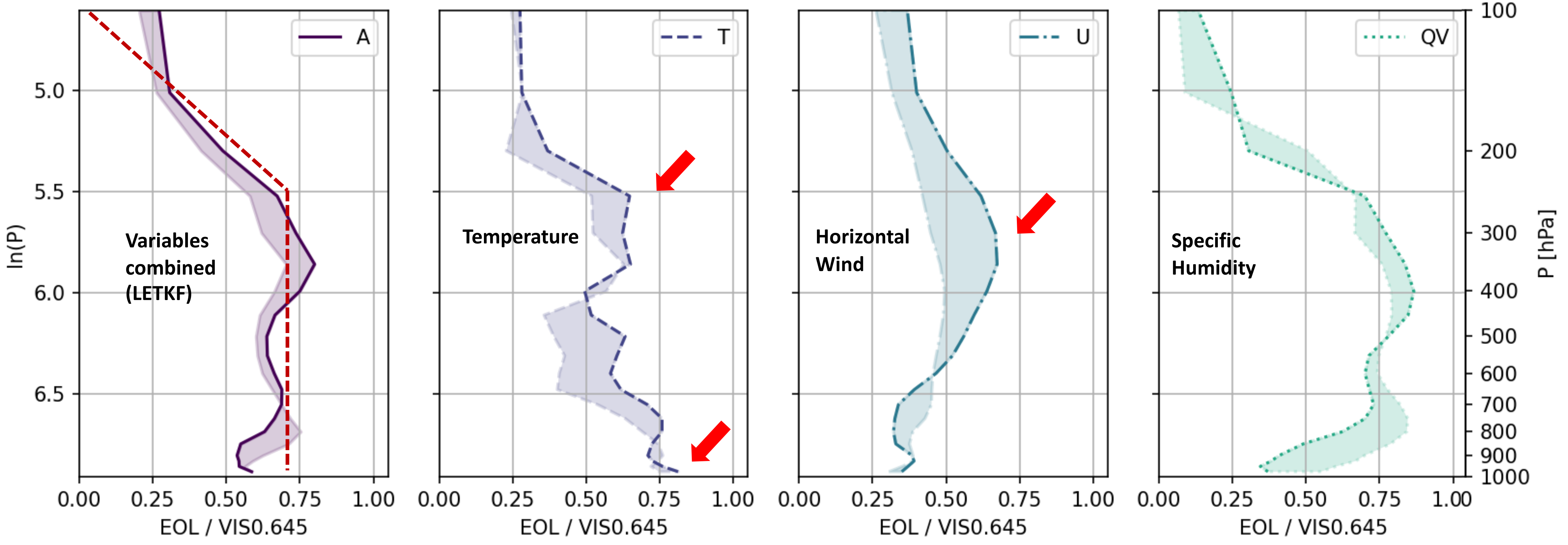
→ **Domain-uniform EOL mainly peaks between 250-400 hPa; Humidity revelas asymmetric localization shape**



IR (band 10 – 7.35 μm) | Solid = Case 1 | Dashed = Case 2 | Shading = Variability

Domain-uniform EOL / Visible 0.64 µm channel

→ **Localization exhibits multiple peaks; VIS 0.6µm strongly correlated with T in lower troposphere / surface levels**

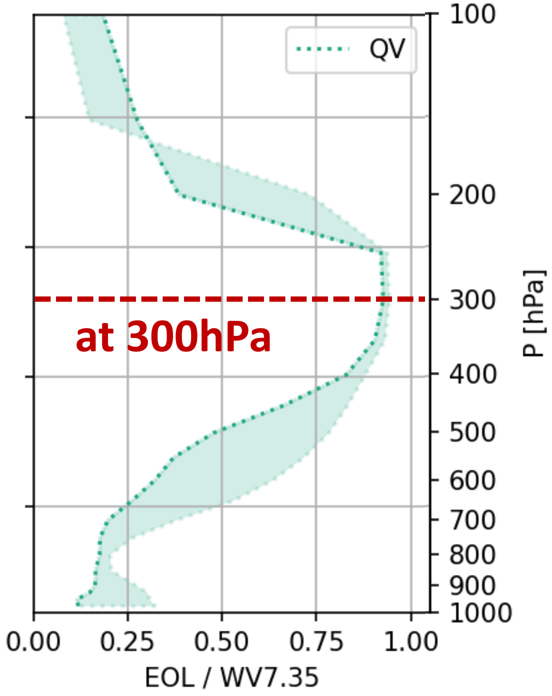


VIS (band 3 – 0.64 µm) | Solid = Case 1 | Dashed = Case 2 | Shading = Variability

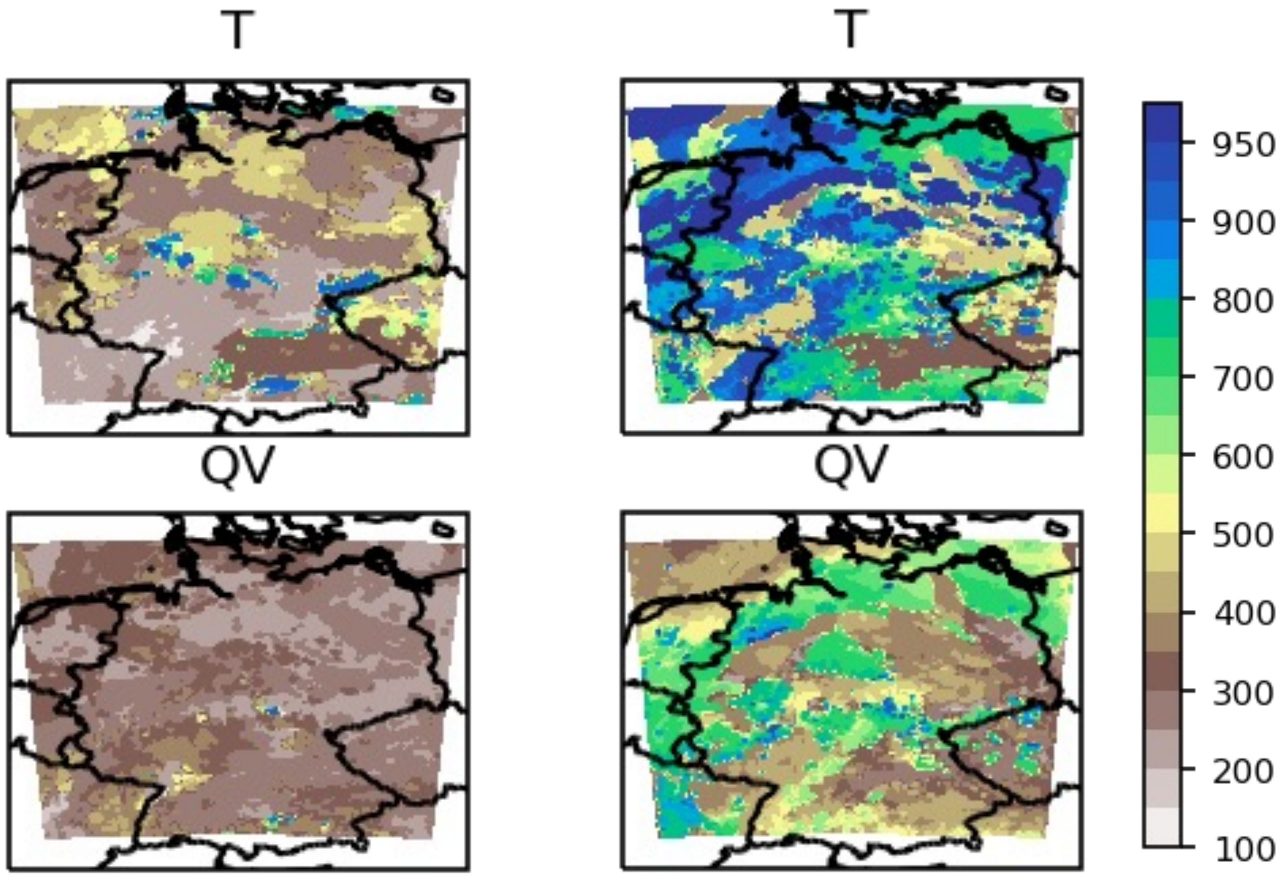
EOL for diagnostics: How situation dependent should localization be?

→ **Visible channels shows higher situation-dependence and would benefit more from adaptive localization**

Diagnostic: Derive level (hPa) of maximum column EOL

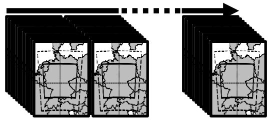


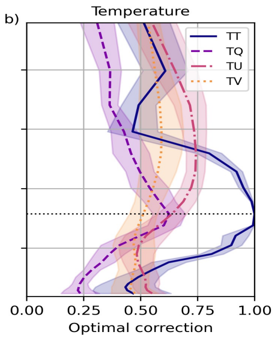
≈ good height estimate of GC center

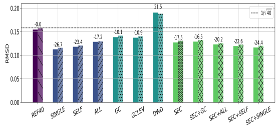


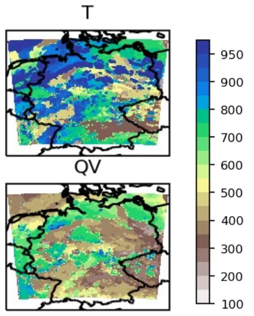
IR (band 10 – 7.35 μm) **VIS** (band 3 – 0.64 μm)

Conclusions – Take away massages









Empirical Optimal Localization (EOL) method allows deriving optimal localization from large ensembles using subsampling

$$\alpha_{single} = \frac{\sum_{s=1}^{S} r_s^{40} r^{1000}}{\sum_{s=1}^{S} (r_s^{40})^2}$$

Vertical model space covariance localization:

- Positive-definiteness: NCM algorithm (Higham, 2002) interesting tool for DA or ML
- Localization shapes, scales and approaches: Variable- and height-dependence
  --> *substantial room for improvements over current GC-based localizations*

Vertical observation space localization of satellite observations:

- Localization should be channel, variable, and cloud situation dependent
- Visible channels benefit more from situation-dependent localization than WV channels

Reference: Necker et al. 2023:
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