Applied Spectroscopy

# Determination of the experimental error of high spectral resolution infrared observations from spectral residuals: application to IASI


- C. Serio[1], G. Masiello[1], C. Camy-Peyret[2], E. Jacquette[3], O. Vandermarcq[3], F. Bermudo[3], D. Coppens[4], D. Tobin[5]

*[1]School of Engineering, University of Basilicata, Potenza, Italy*
*[2]IPSL (UPMC/UVSQ) Paris, France*
*[3]CNES, Toulouse, France*
*[4]EUMETSAT, Darmstadt, Germany*
*[5]CIMMS/SSEC, University of Wisconsin, Madison, USA*

# Background

1. The problem of how to characterize instrument noise directly from observed radiances has received a deal of attention in the past years. Most studies address the problem with heuristic or empirical approaches.

2. In contrast, our analysis is based on a firm statistical approach, which leaves no room to ad hoc assumptions.

3. Our methodology does not address the problem of forward model noise (that is the noise due to instrument and forward model uncertainty and bias), which is the topics of many concurrent studies.

4. We are focused on the instrument noise alone.

# We are focused on the instrument noise alone and have developed two tools, which will be exemplified through application to IASI

## A forward model based approach

5924 Vol. 54, No. 19 / July 1 2015 / Applied Optics Research Article

applied optics

**Infrared atmospheric sounder interferometer radiometric noise assessment from spectral residuals**

Carmine Serio,[1,2,*] Carsten Standfuss,[3] Guido Masiello,[1,2] Giuliano Liuzzi,[1] Emmanuel Dufour,[3] Bernard Tournier,[3] Rolf Stuhlmann,[4] Stephen Tjemkes,[4] and Paolo Antonelli[5]

[1]Scuola di Ingegneria, Universitá della Basilicata, Potenza 85100, Italy
[2]CNISM, Unitá di Ricerca Universitá della Basilicata, Potenza 85100, Italy
[3]Noveltis, Labege 31670, France
[4]EUMETSAT, Darmstadt 64295, Germany
[5]SSEC, University of Wisconsin, Madison, Wisconsin 53706, USA
*Corresponding author: carmine.serio@unibas.it

## A PCA/BIC based approach

Journal of Quantitative Spectroscopy & Radiative Transfer 206 (2018) 8–21

Contents lists available at ScienceDirect

ELSEVIER

Journal of Quantitative Spectroscopy & Radiative Transfer

journal homepage: www.elsevier.com/locate/jqsrt

**PCA determination of the radiometric noise of high spectral resolution infrared observations from spectral residuals: Application to IASI**

CrossMark

C. Serio[a,*], G. Masiello[a], C. Camy-Peyret[b], E. Jacquette[c], O. Vandermarcq[c], F. Bermudo[c], D. Coppens[d], D. Tobin[e]

[a] Scuola di Ingegneria, Università della Basilicata, Potenza, Italy
[b] Institut Pierre-Simon Laplace (IPSL), UPMC/UVSQ, Paris, France
[c] CNES, Toulouse, France
[d] EUMETSAT, Darmstadt, Germany
[e] CIMMS/SSEC, University of Wisconsin, Madison, USA

# Both Approaches rely on the concept of spectral residuals

## FM based approach

- $\delta \boldsymbol{R} = \boldsymbol{R}_{obs} - F(\boldsymbol{v})$,
- $F$, the forward model
- $\boldsymbol{v}$, the state vector estimated based on a suitable retrieval procedure

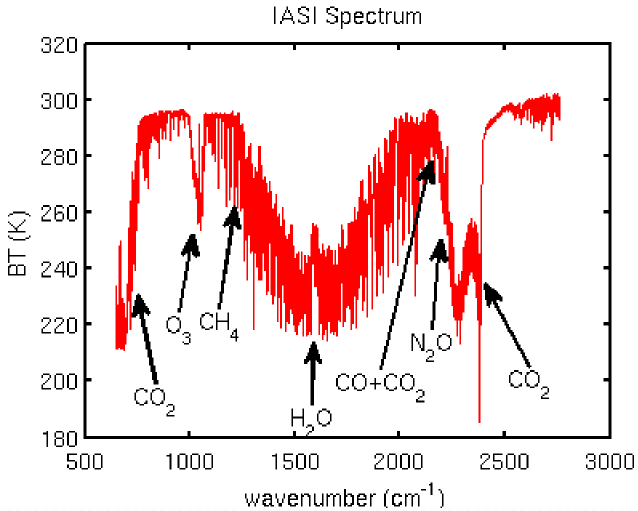
- After a proper localization, the instrument noise covariance matrix is estimated by

- $\widehat{\boldsymbol{S}}_{\varepsilon} =< (\delta \boldsymbol{R} - \overline{\delta \boldsymbol{R}})(\delta \boldsymbol{R} - \overline{\delta \boldsymbol{R}})^{t} >$

## PCA approach

- After appropriate centering of the radiance vector,
- $\delta \boldsymbol{R} = \boldsymbol{R}_{obs} - \boldsymbol{U}_{\tau} \boldsymbol{c}$
- $\boldsymbol{U}$ orthogonal basis of PCA $\boldsymbol{c}$ vector, truncated at $\tau$
- For a given $\tau$ and a-priori normalizing covariance, $\widetilde{\boldsymbol{S}}_{\varepsilon}$, the instrument noise covariance is estimated by
- $\widehat{\boldsymbol{S}}_{\varepsilon} = \widetilde{\boldsymbol{S}}_{\varepsilon}^{1/2} \boldsymbol{U}_{-\tau} \boldsymbol{\Lambda} \boldsymbol{U}_{-\tau}^{t/2} \widetilde{\boldsymbol{S}}_{\varepsilon}^{t/2}$
- with $\boldsymbol{\Lambda}$ the diagonal matrix of eigenvalues,
- $\widetilde{\boldsymbol{S}}_{\varepsilon}$ is the full IASI covariance matrix according to the EUMETSAT/CNES release.

For both approaches, we use the whole IASI spectral coverage (8461 channels). The FM approach is combined with Random Projections and we simultaneously retrieve parameters and gas species. (Poster 8p.02)

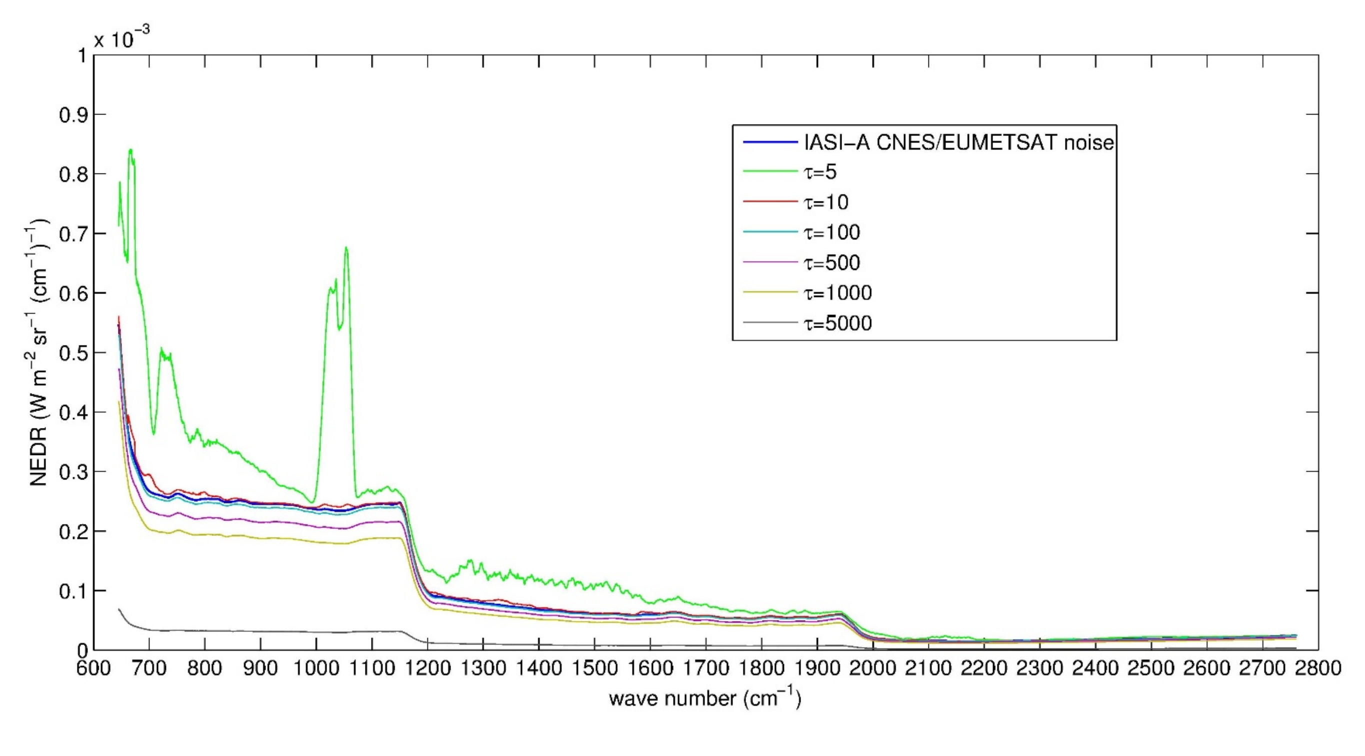



Retrieved parameters and species include

- Surface
  - Temperature
  - Emissivity (spectrum)
- Atmospheric Profiles of
  - Temperature
  - $H_2O$
  - $O_3$
  - HDO
  - $CO_2$
  - $N_2O$
  - CO
  - $CH_4$
  - $SO_2$
  - $HNO_3$
  - $NH_3$
  - OCS
  - $CF_4$

# PCA approach; application to IASI A: simulation

**The PCA approach estimator is fully analytical, we do not need for each truncation point $\tau$ to re-compute the spectral residuals. However it critically depends on the given $\tau$ and the estimator is biased**



# Develop an approach, which simultaneously and optimally estimates noise and truncation point

**Step 1**: Write the PCA problem in a probabilistic fashion using the formalism of latent variables

$$\boldsymbol{x} = \boldsymbol{Hw} + \boldsymbol{\eta}$$

**Step 2**: Define a log-likelihood cost function

$$\mathcal{L} = \frac{\boldsymbol{N}}{\mathbf{2}}\left(d\log(\mathbf{2}\boldsymbol{\pi}) + \log(|\boldsymbol{S}_{\boldsymbol{x}}|) + \mathbf{tr}(\boldsymbol{S}_{\boldsymbol{x}}^{-1}\boldsymbol{S})\right)$$

**Step 3**: Compute the Bayesian Information Criterion, BIC and get the optimal solution by seeking for BIC minimum

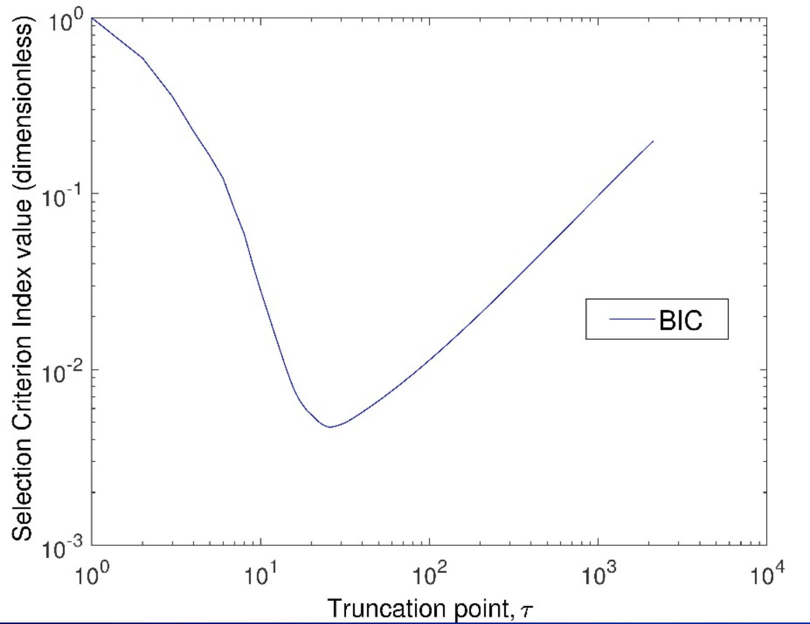
$$\boldsymbol{BIC} = -\mathbf{2}\log \boldsymbol{p}(\boldsymbol{x}|\boldsymbol{\tau})$$

Gideon Schwarz, Estimating the Dimension of a Model, Ann. Statist. Volume 6, Number 2 (1978), 461-464.

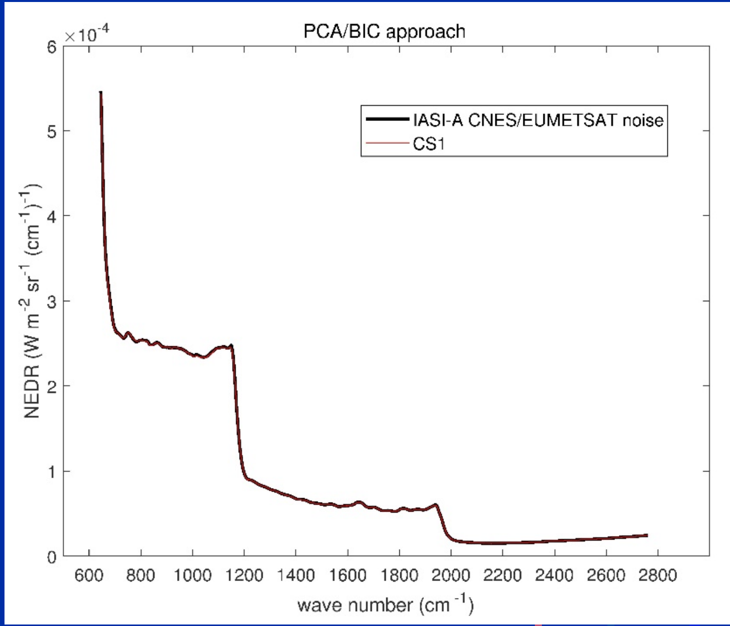
$$\begin{aligned}\mathrm{BIC}(\tau) &= -2\log\left(p(\mathbf{X}|\tau)\right) \\ &= N\sum_{j=1}^{d}\log\lambda_j + N(d-\tau)\log\left(\frac{1}{d-\tau}\sum_{j=\tau+1}^{d}\lambda_j\right) \\ &+ (\tau+k)\log N\end{aligned}$$

# PCA/BIC approach, application to IASI in simulation

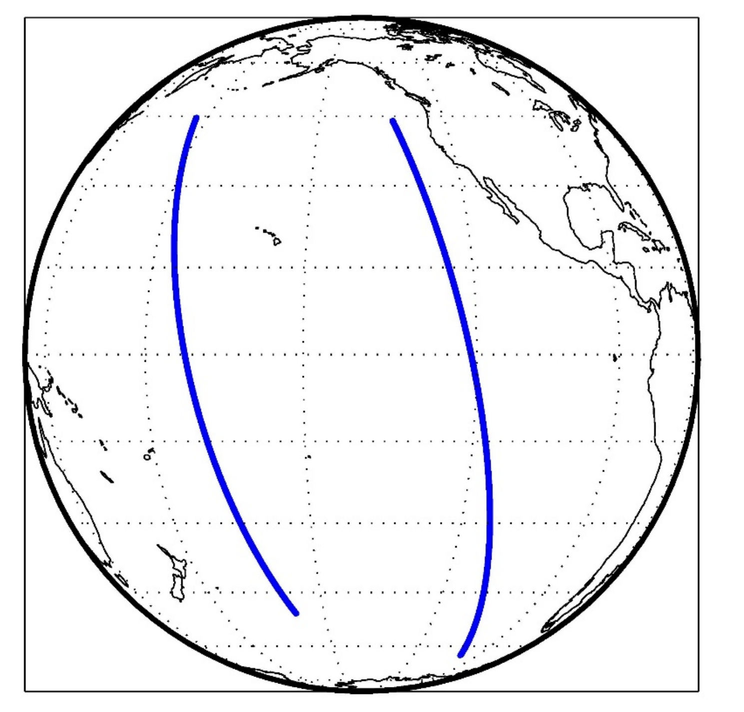
## Seek for BIC minimum



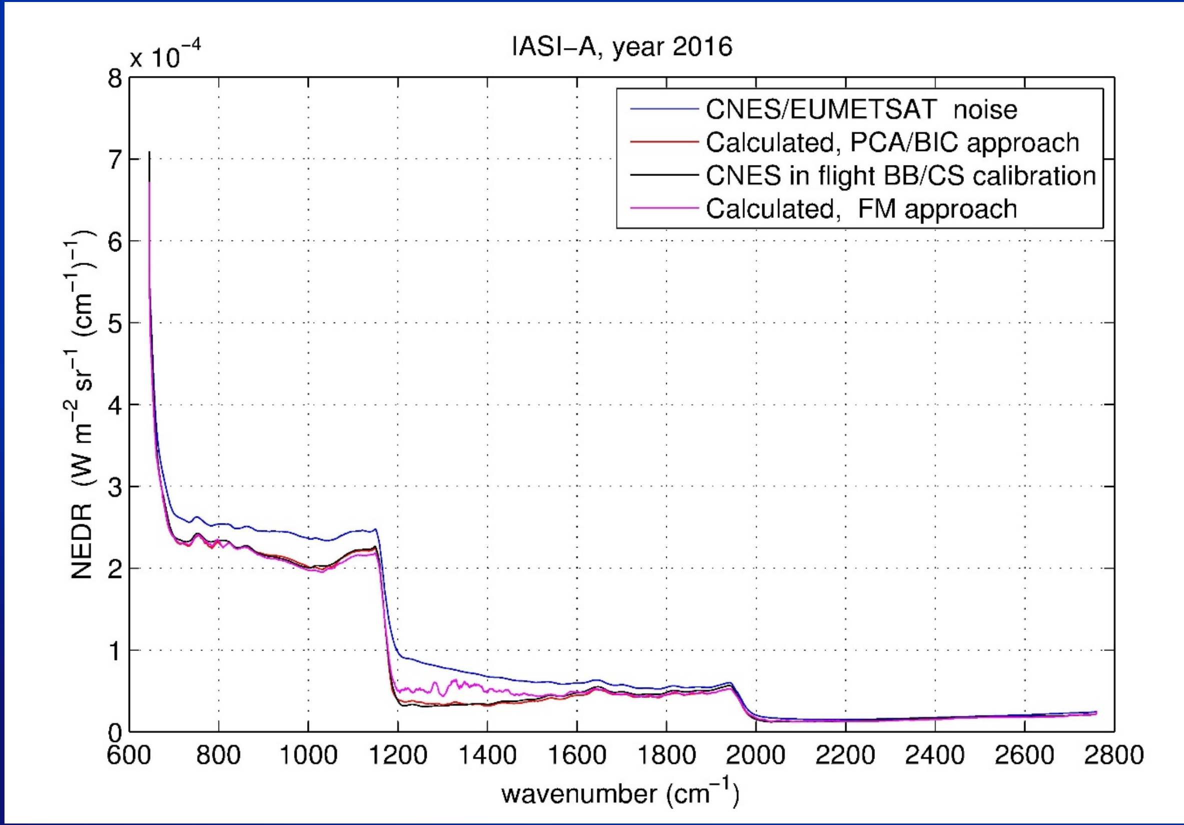

## Estimated radiometric noise at the BIC minimum, $\tau = 26$



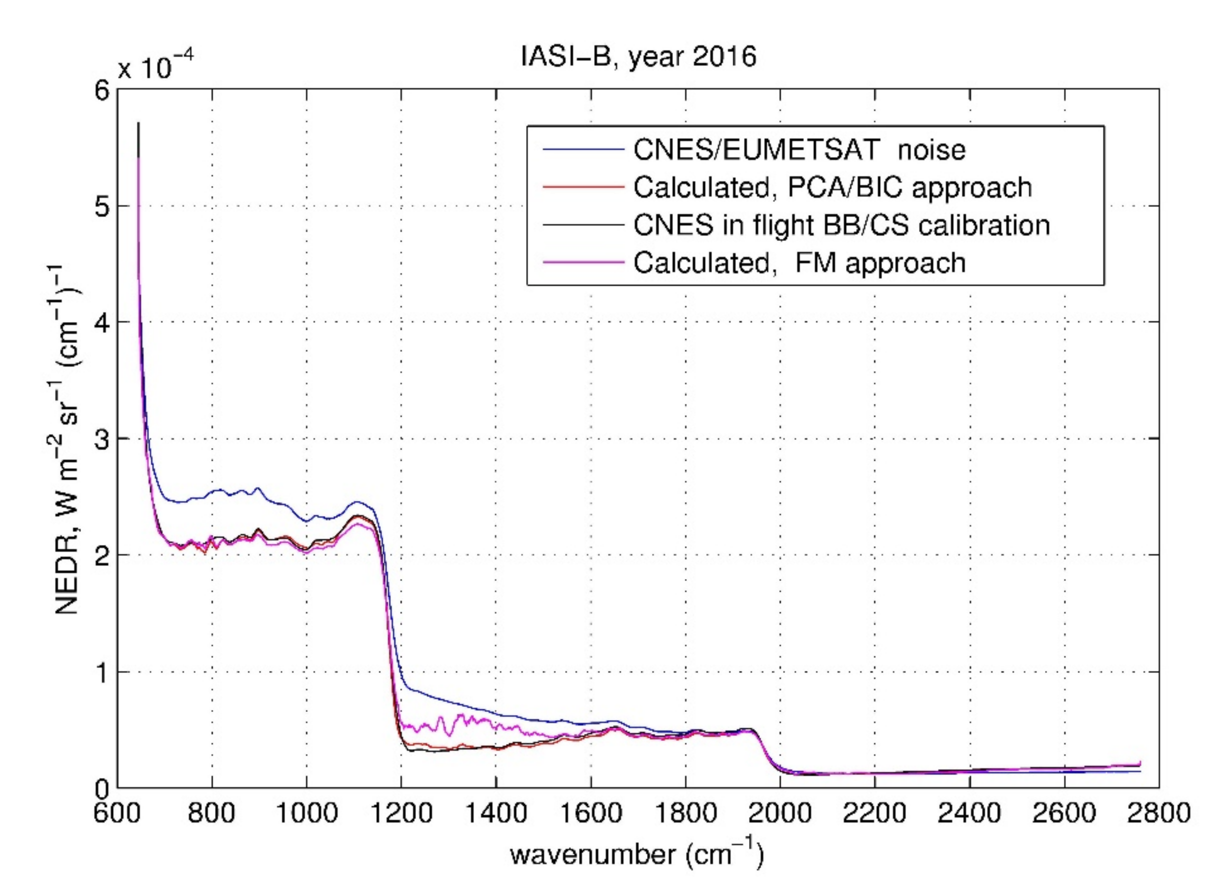
# Application to IASI: IASI data in external calibration (ExtCal) mode for the year 2016



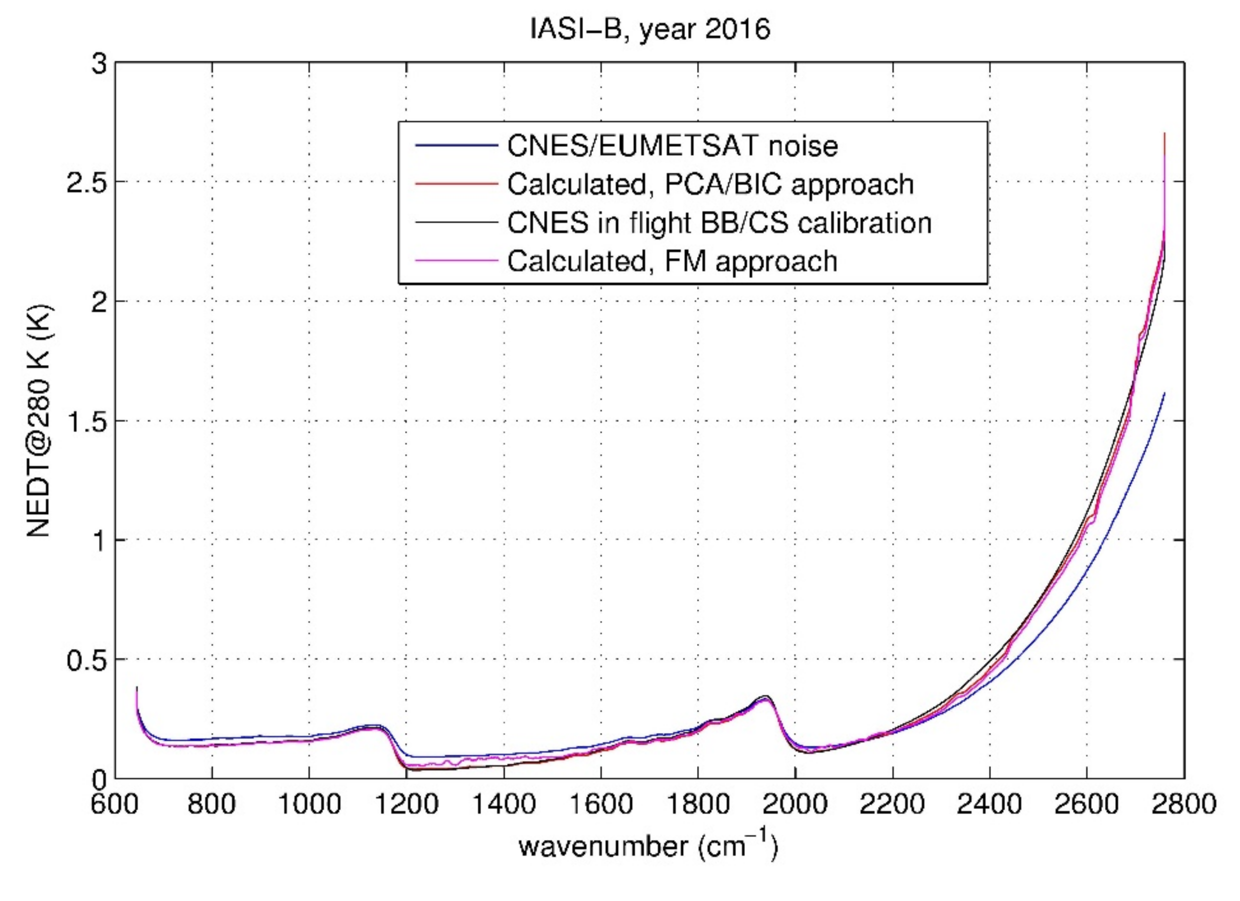
# IASI-A, PCA/BIC perfectly matches BB in flight calibration. Data averaged over the whole year 2016



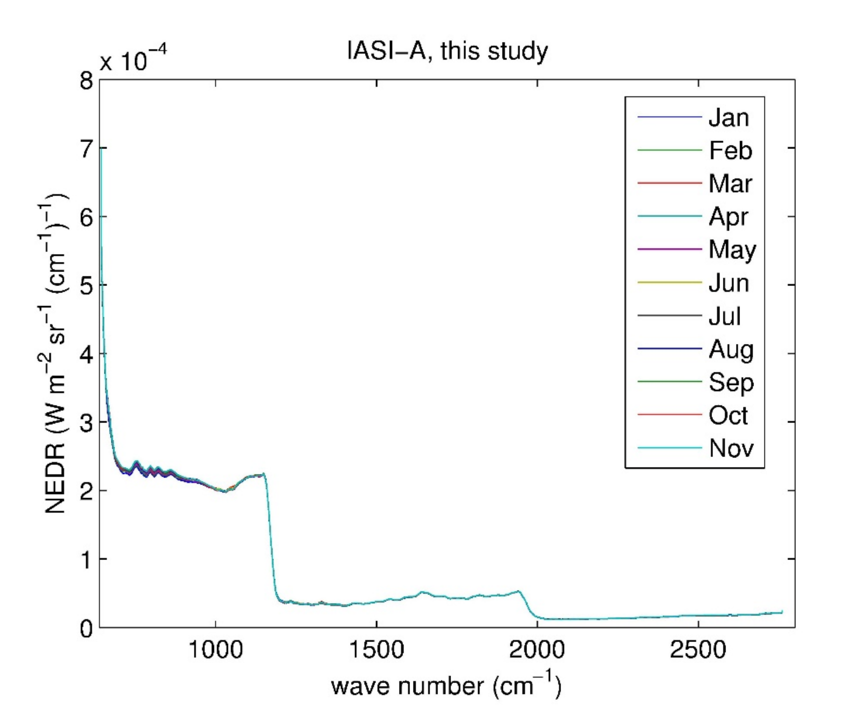
# IASI-B, PCA/BIC perfectly matches BB in flight calibration. Data averaged over the whole year 2016

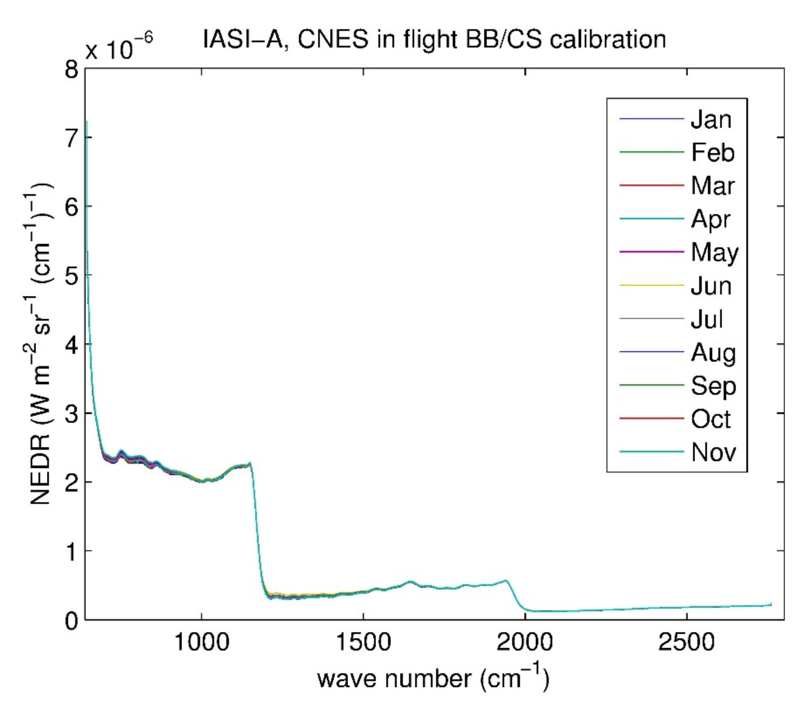


# IASI-B, PCA/BIC perfectly matches BB in flight calibration. Data averaged over the whole year 2016. NEDT Analysis

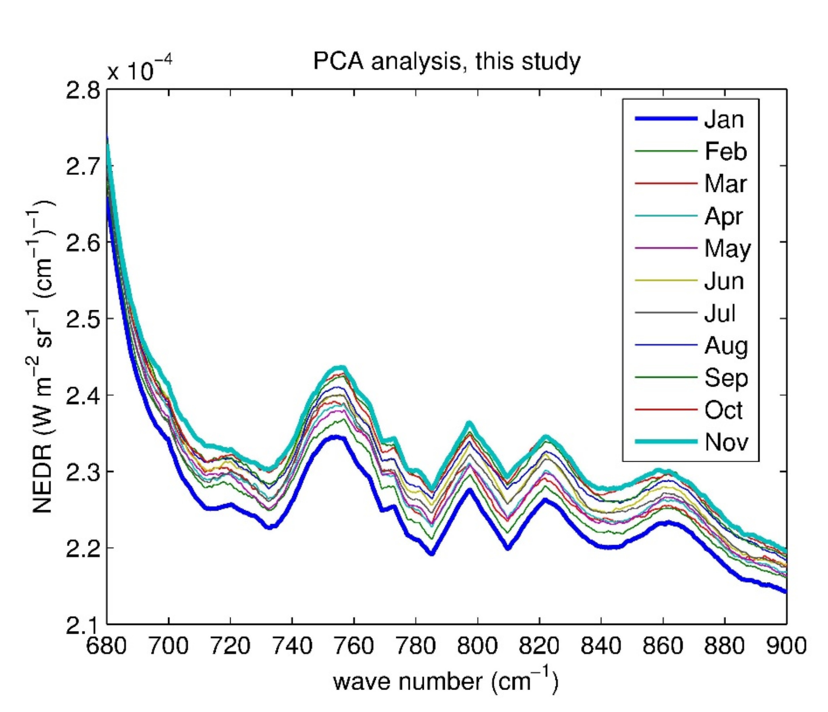


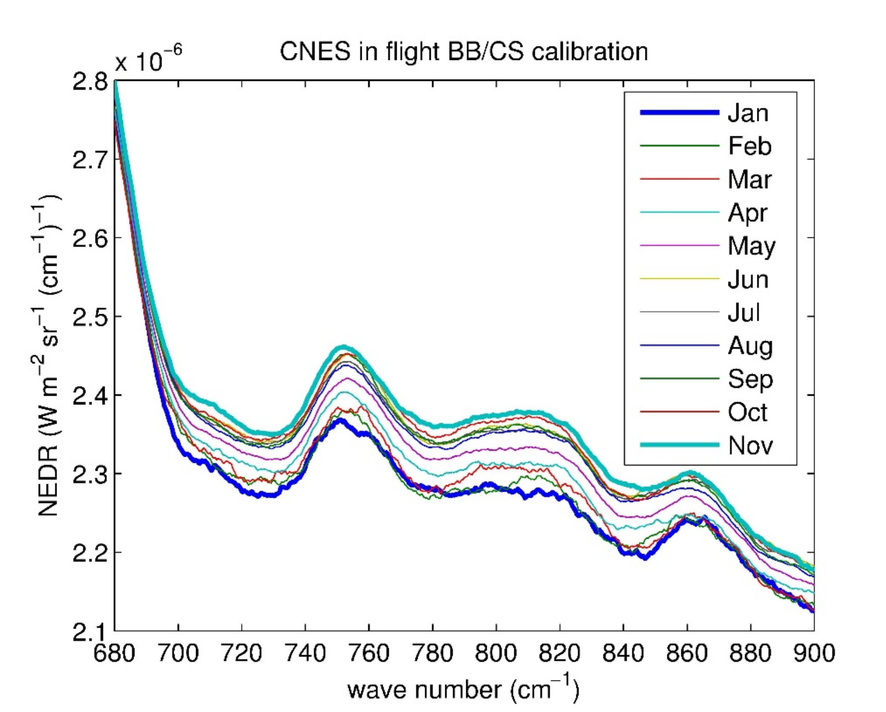
# Radiometric noise as a function of month. The case of IASI-A



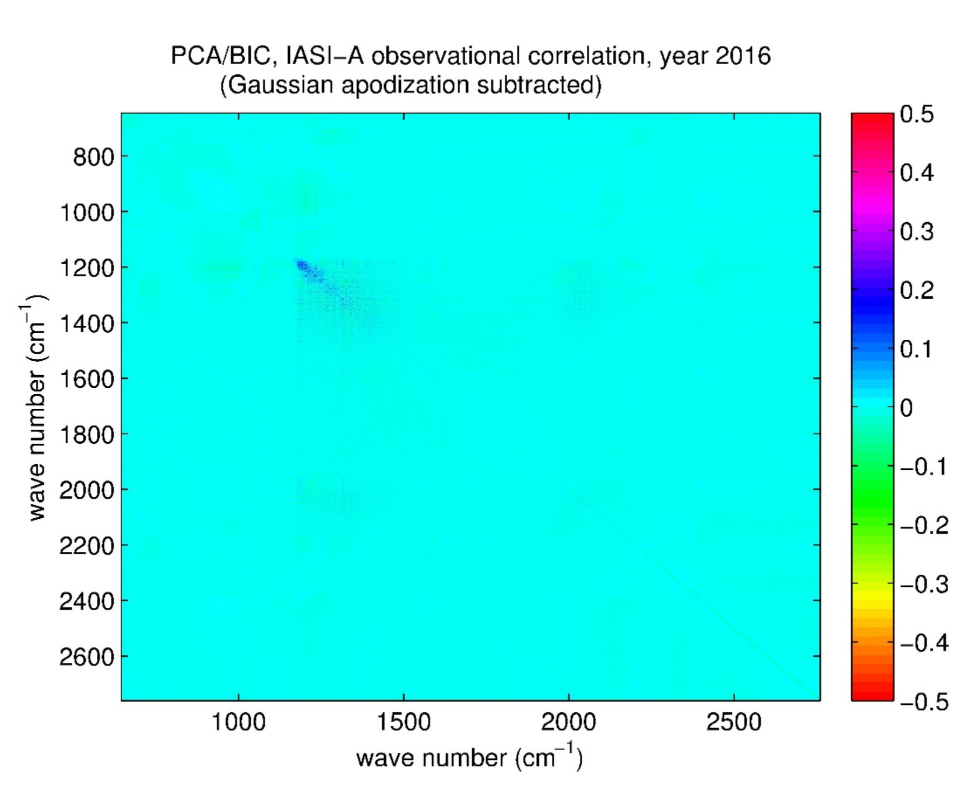



# Radiometric noise as a function of month. The case of IASI-A. PCA/BIC can track differences as small as that due to icing



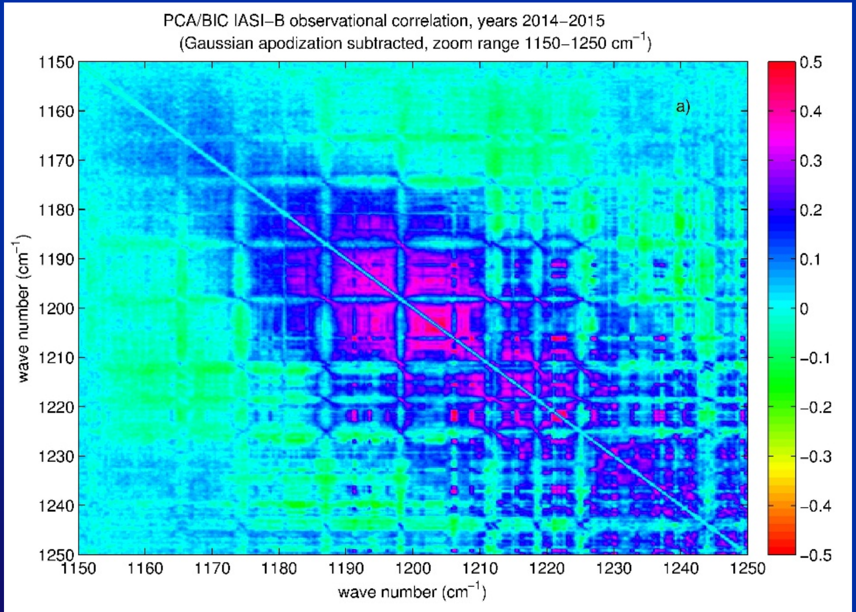



# COVARIANCE MATRIX, IASI-A

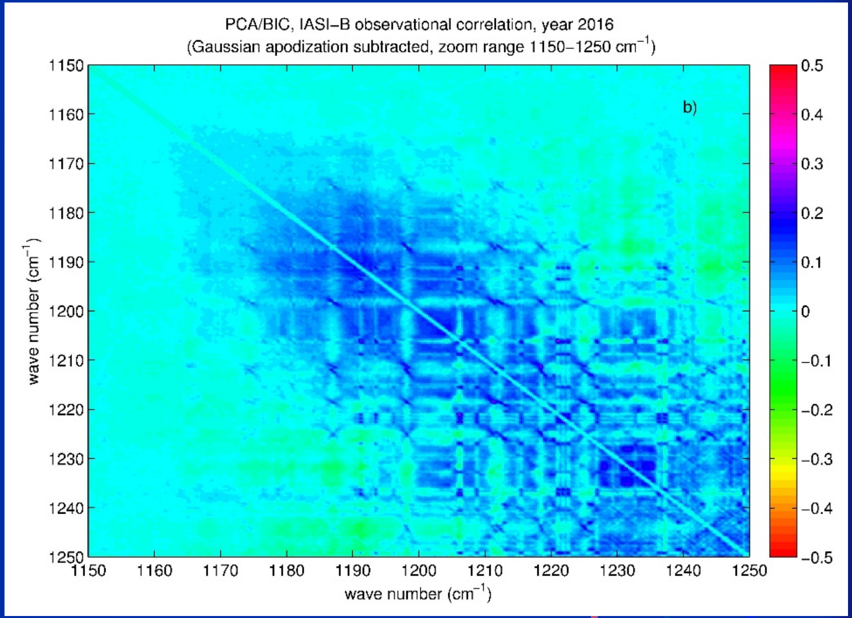


# IASI-A, comparison CD ON vs CD OFF

## CD ON

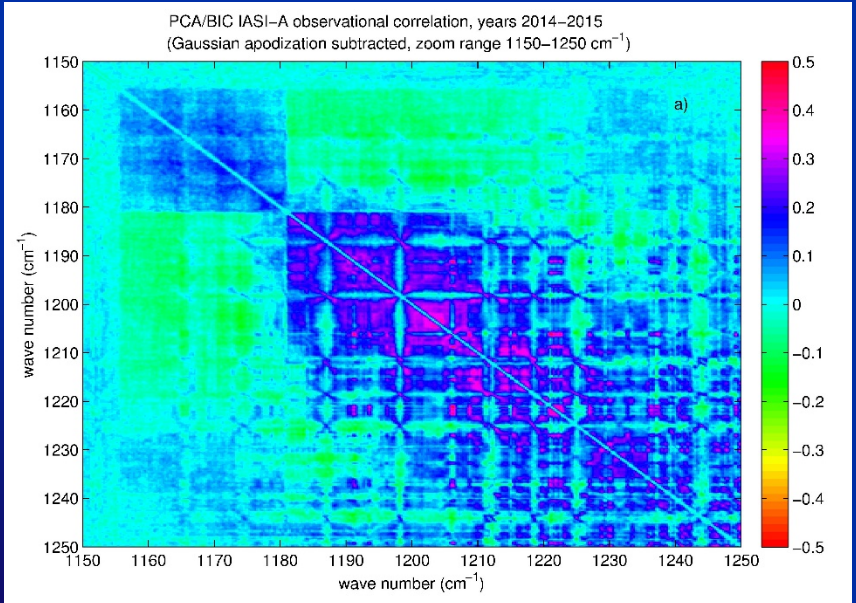



## CD OFF

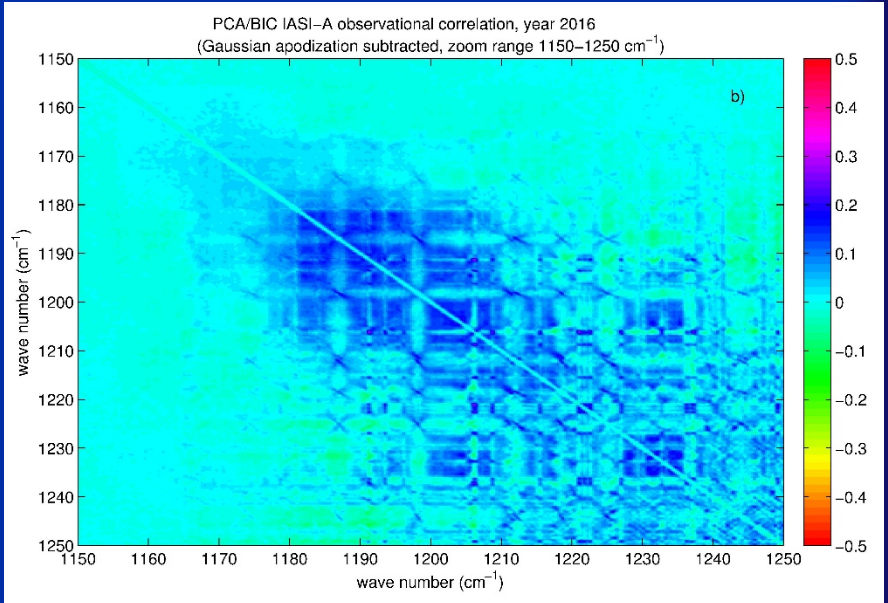


# IASI-B, comparison CD ON vs CD OFF

## CD ON




## CD OFF



# Conclusions

- IASI is spectrally and radiometrically stable. The spectral quality has improved after switching off the CD mechanism.
- The FM and PCA/BIC approaches complete each other, the PCA/BIC is much faster.
- There are a lot of lessons learned by applying the PCA/BIC, which, e.g., are important for PCA compression,
  - In case of IASI, the normalization to the diagonal of the covariance matrix yields the worst results, the dimensionality is artificially increased! Normalization to the diagonal is even worse than not considering normalization at all. The best way to normalize is to use the correct covariance matrix we have estimated with the PCA/BIC approach.
- In addition, the IASI covariance provided by us should be used when IASI is used for spectroscopy.
- We are planning to apply PCA/BIC methodology to AIRS, CrIs, possibly FY-A4 and hopefully ESA-Forum Mission Explorer in the far infrared.