

# PCA based information content studies from high spectral resolution infrared observations



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# Questions we are trying to answer

- ◆ What is the impact of PCA on hyperspectral IR data?
  - Estimation of the Information Loss
  - Noise reduction
- ◆ What do the Principal Components represent?
  - Statistical meaning
  - Physical meaning
- ◆ What are the benefits and risks in applying PCA to hyperspectral IR data for noise filtering?
  - How should it be applied?
  - When should it be applied?

# Outline

- PCA used to Filter out random component of instrument Noise (PNF)
  - Theory
- Application of PNF to simulated data
  - Aircraft FTS data
- Application of PNF to real data
  - Airborne FTS and Spaceborne Grating observations
- Conclusions

# Noise Filter Problem

$$L_{\text{obs}}(\mathbf{v}) = L_{\text{atm}}(\mathbf{v}) + \eta(\mathbf{v})$$

Find F such that:  $L_{\text{est}}(\mathbf{v}) = F(L_{\text{obs}}(\mathbf{v}))$

With minimal Estimation Errors:  $EE(\mathbf{v}) = L_{\text{est}}(\mathbf{v}) - L_{\text{atm}}(\mathbf{v})$

If  $S = \text{cov}(\eta)$  and  $R = \text{cov}(L_{\text{atm}})$  are known,  
the optimal linear filter in the least square sense is

$$F = R(R + S)^{-1}$$

MMSE

PCA

$$L_{\text{est}}(\mathbf{v}) = P(L_{\text{obs}}(\mathbf{v}))$$

# Useful Quantities

Estimation Error (**EE**): difference between noise free and filtered signals

Atmospheric Information Loss (**AIL**): difference between noise free signal before and after filtering

Reconstructed Noise (**RN**): noise signal after filtering

Reconstruction Residuals (**RR**): difference between observed signal before and after filtering

# PCA Noise Filter: Implementation Strategy

- Normalize each spectrum  $L_{\text{obs}}$  by estimated Noise Equivalent Radiance
- Derive the Principal Components from observations (Eigenfunctions of Covariance Matrix of **dependent**  $L_{\text{obs}}$ )
- Project each  $L_{\text{obs}}$  onto PCs
- Estimate noise normalized signal ( $L_{\text{est}}$ ) by retaining only  $N_t$  PCs
- Remove normalization

# Noise Reduction Factor (NRF)

After Noise Normalization data:  $\sigma_i=1 \quad \forall i$

Original space:  $\Phi^2 = \sum_{j=1, \dots, N} \sigma_j^2 = N$

Reduced space:  $\Gamma^2 = \sum_{j=1, \dots, N_t} \sigma_j^2 = N_t$

Noise Reduction Factor (NRF)

$$\text{NRF} = \sqrt{\Phi^2 / \Gamma^2} = \sqrt{N / N_t}$$

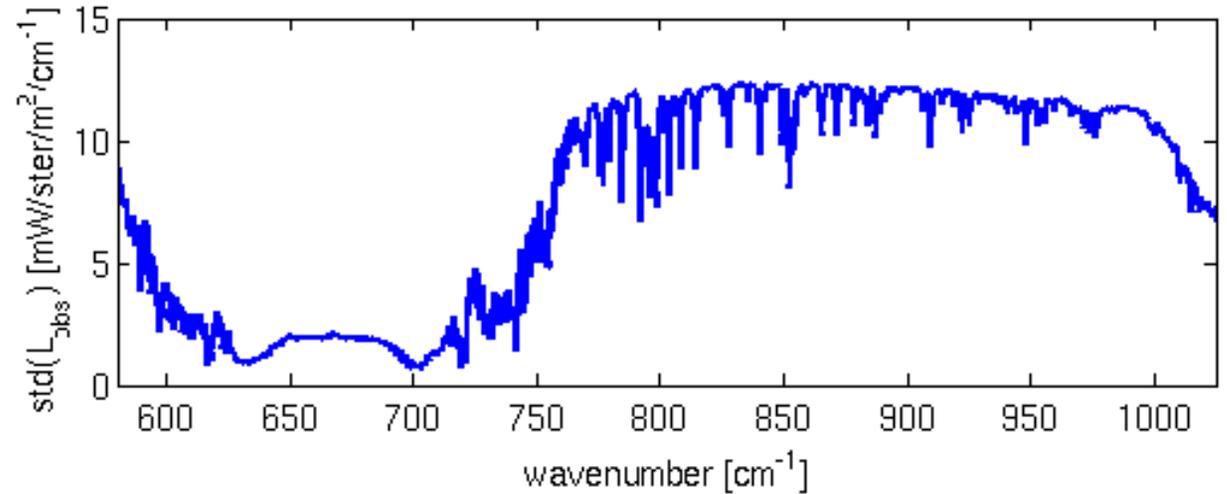
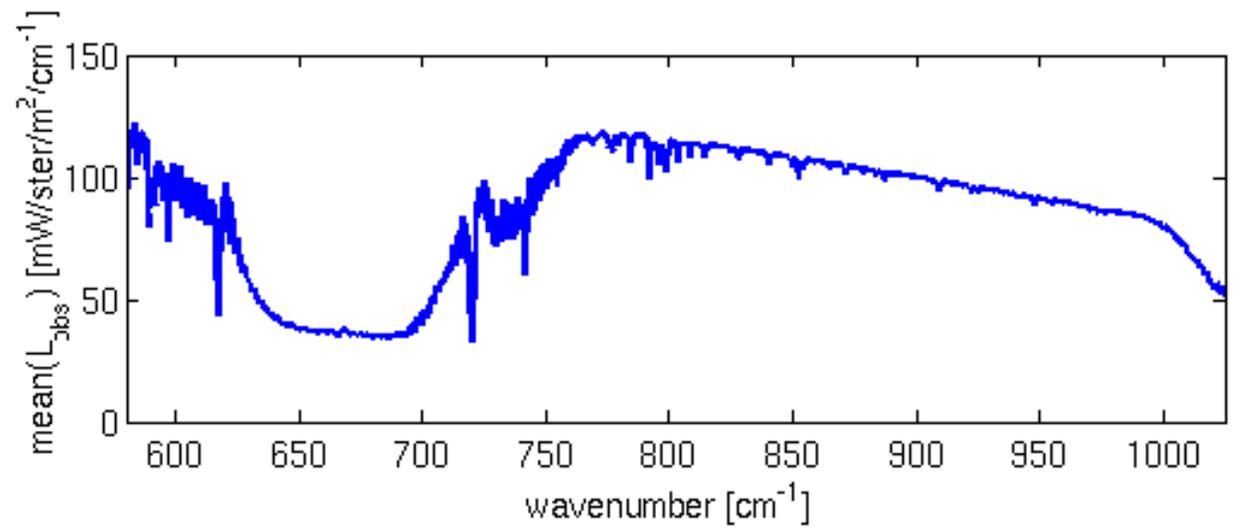
# PNF on Simulated Data

- Quantification of:
  - Atmospheric Information Loss (AIL)
  - Reconstructed instrument Noise (RN)
- Comparison between:
  - Accuracy of PNF (PCA Noise Filter)
  - Accuracy of MMSE (Minimum Mean Square Error from Estimation Theory)
- Verification importance of:
  - Noise normalization
  - Importance of large training sets

# Training Set

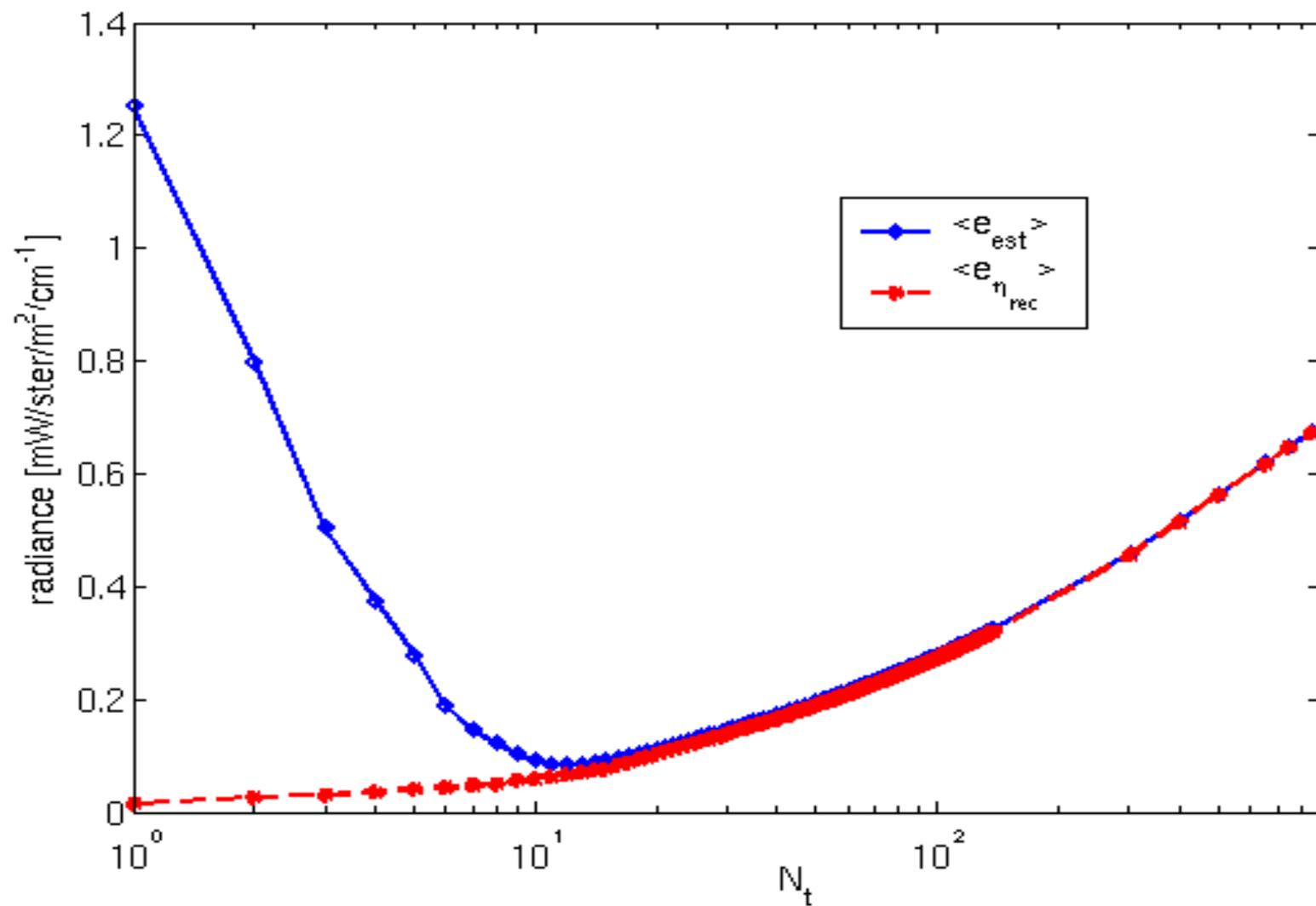
- 10000 raob profiles collected over South Africa (REGIONAL or Local DATASET)
- Clear Sky radiances only, simulated with LBLRTM 8.1 and convoluted at Scanning-HIS resolution (.5  $\text{cm}^{-1}$ )
- Noise RMS estimated from observed instrument noise (Scanning-HIS, 7 Sep 2000)

# Training Set Simulated Data

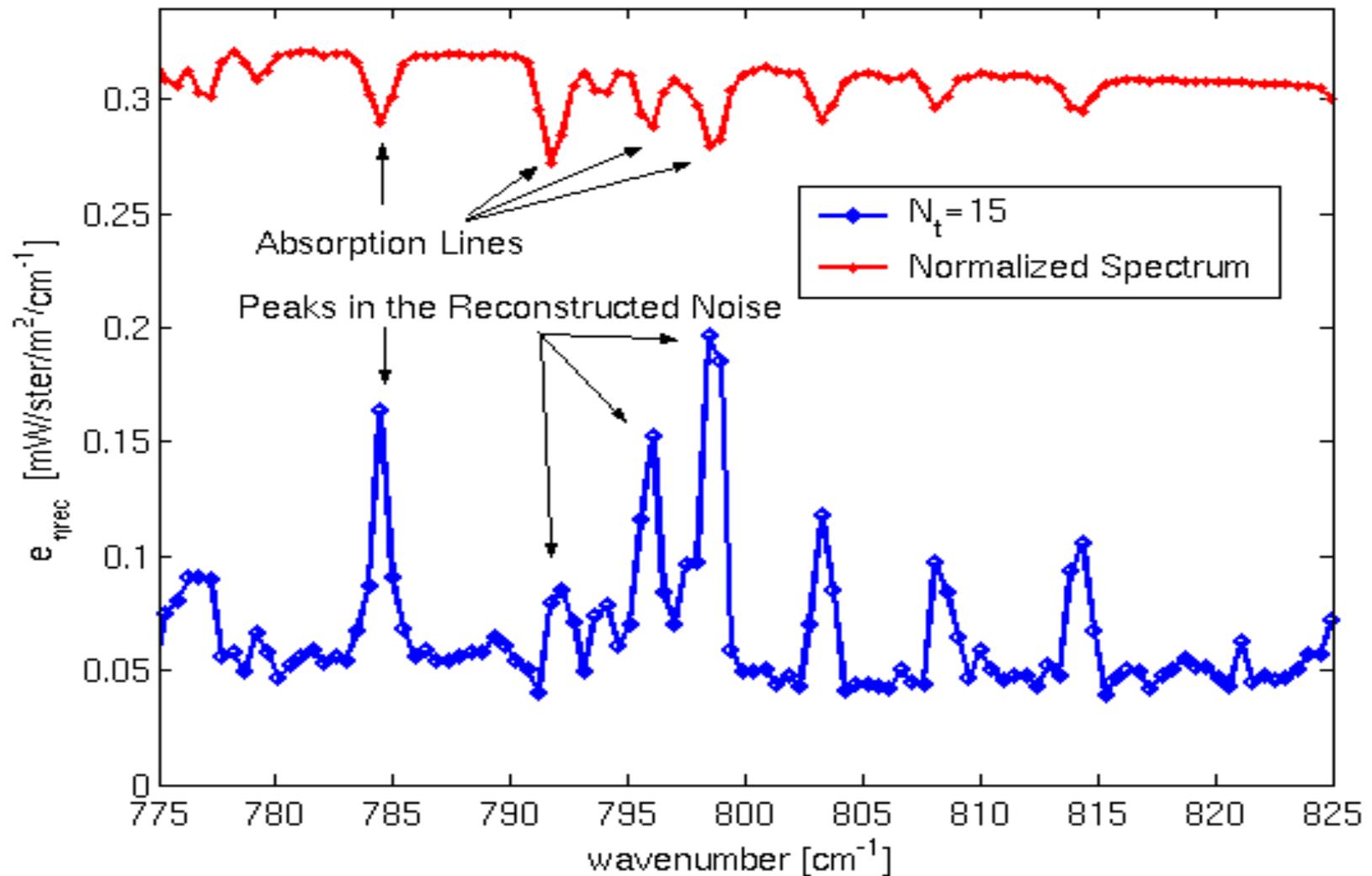


**REGIONAL TRAINING SET**  
July-October / 1990-2000  
Over South-East African Countries

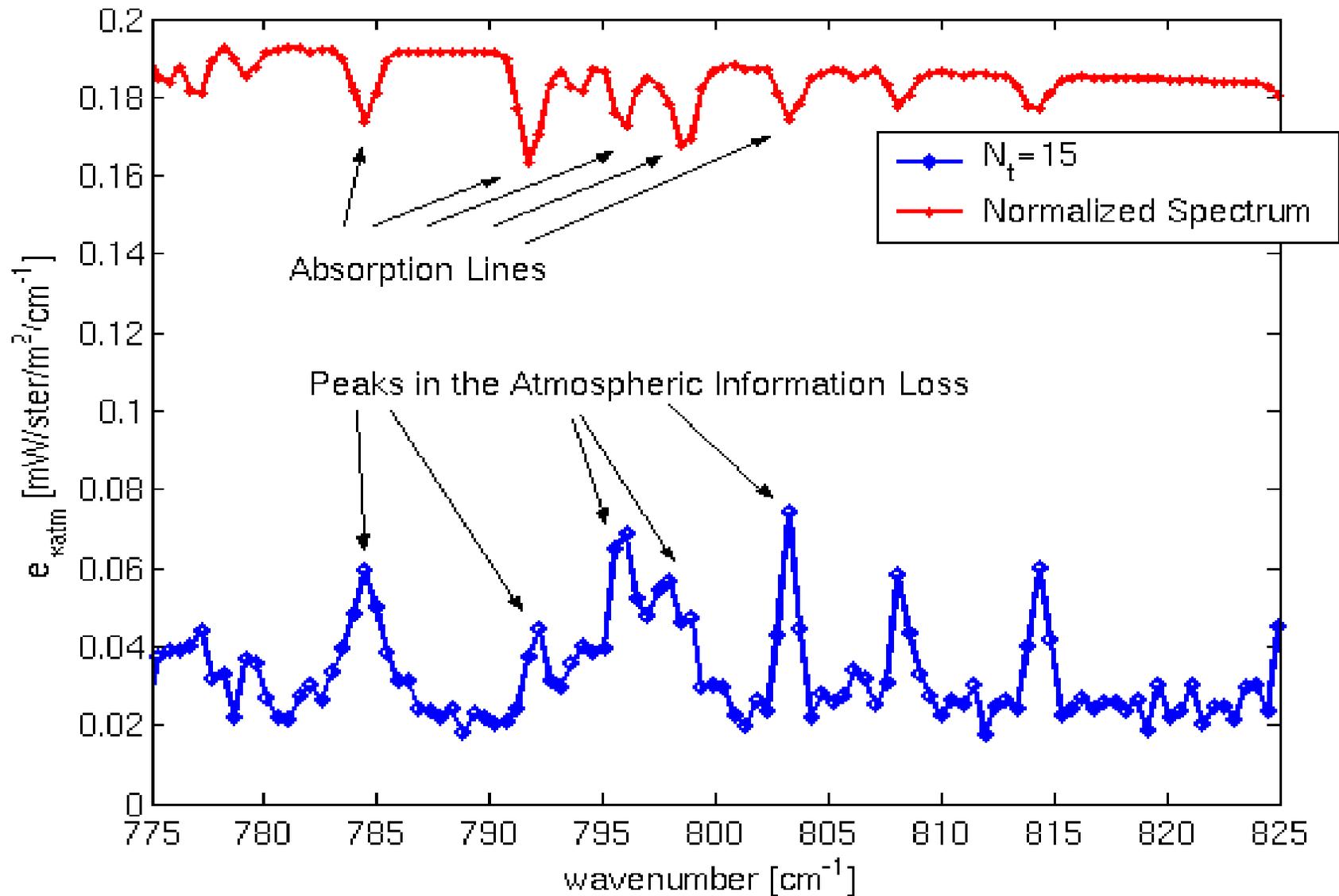
# EE vs RN

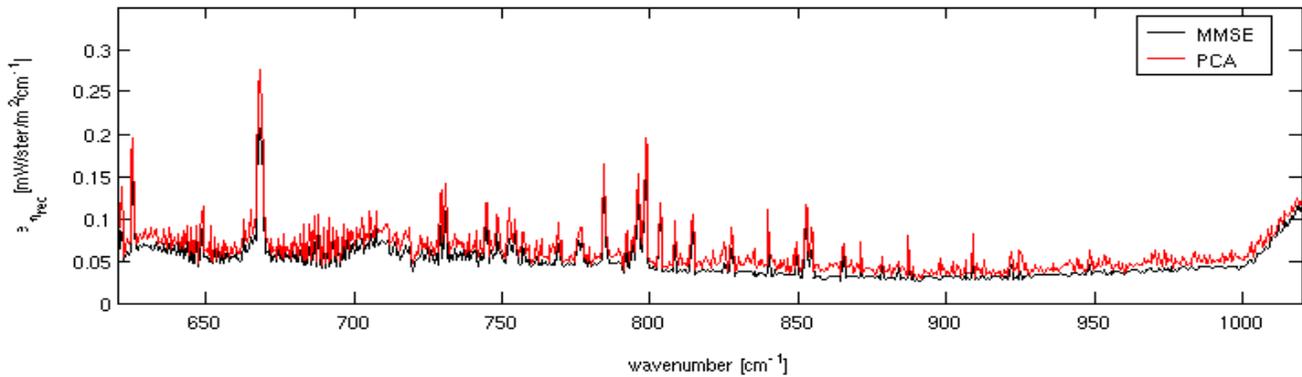


# Correlation in RN



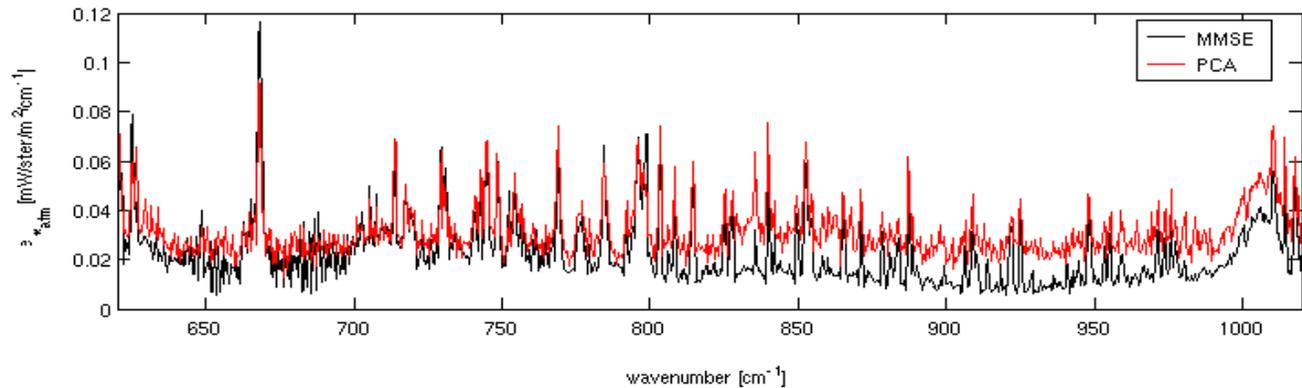
# Correlation in AIL





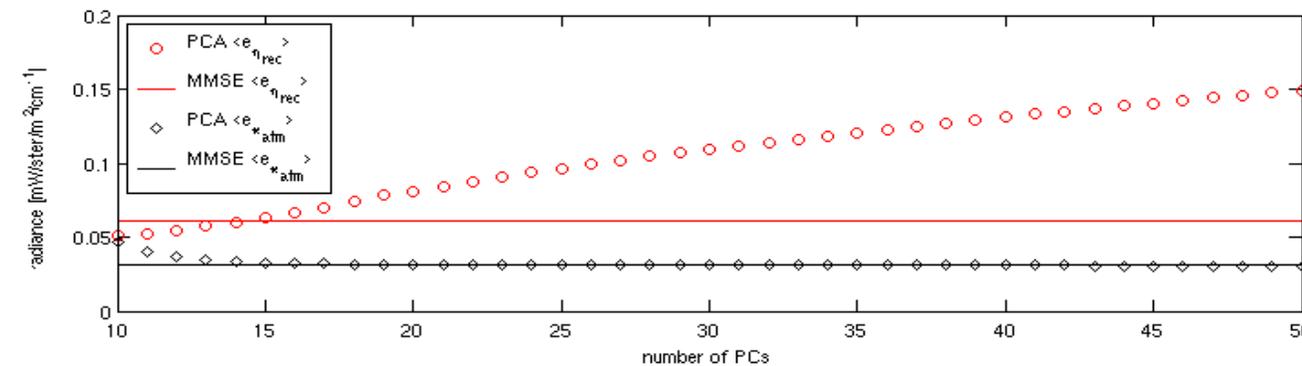
PCA  
Rms(RN)

PCA  
Rms(RN)



PCA  
Rms(AIL)

PCA  
Rms(AIL)

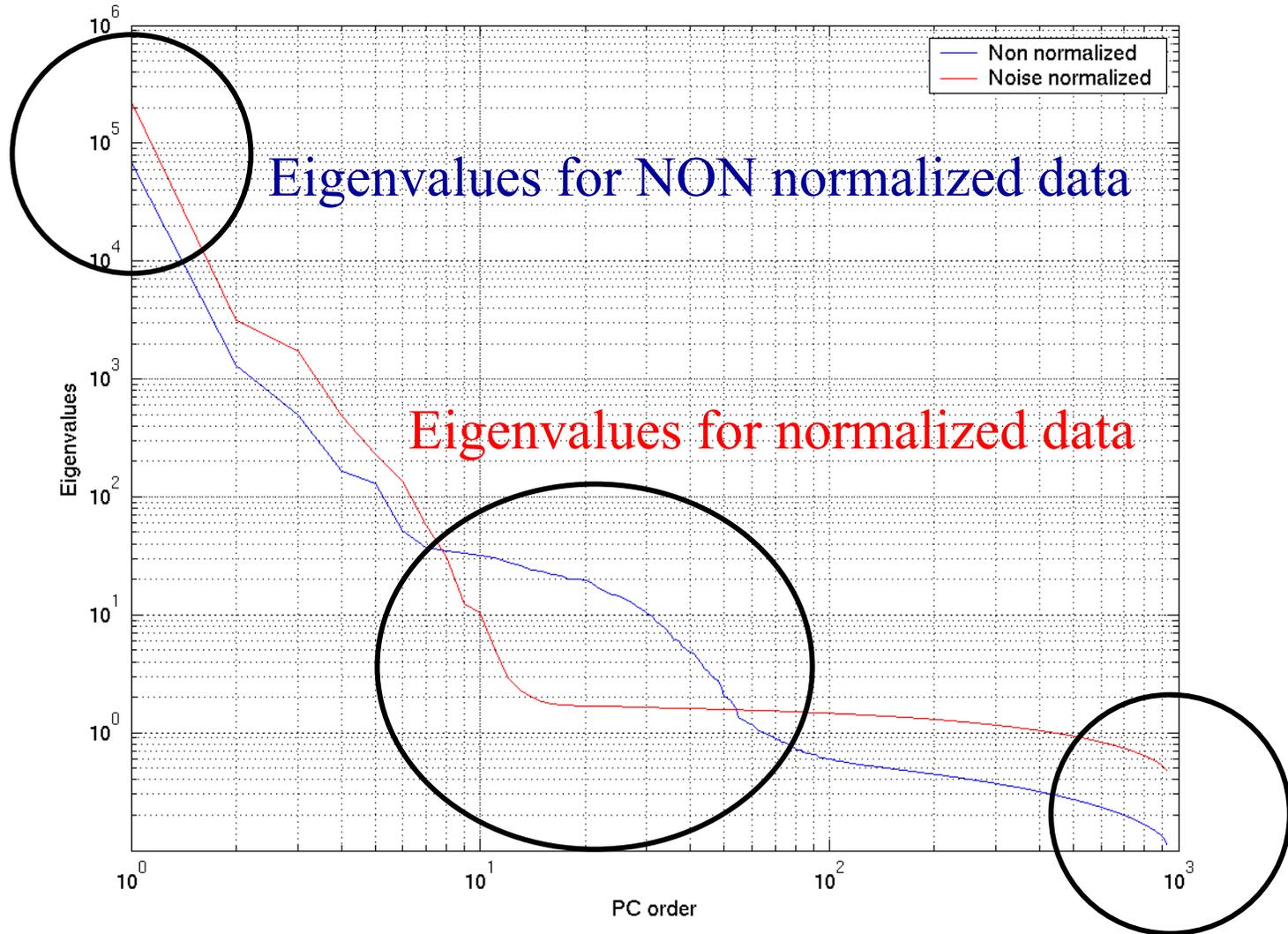


$\langle$ Rms(AIL) $\rangle$

$\langle$ Rms(RN) $\rangle$

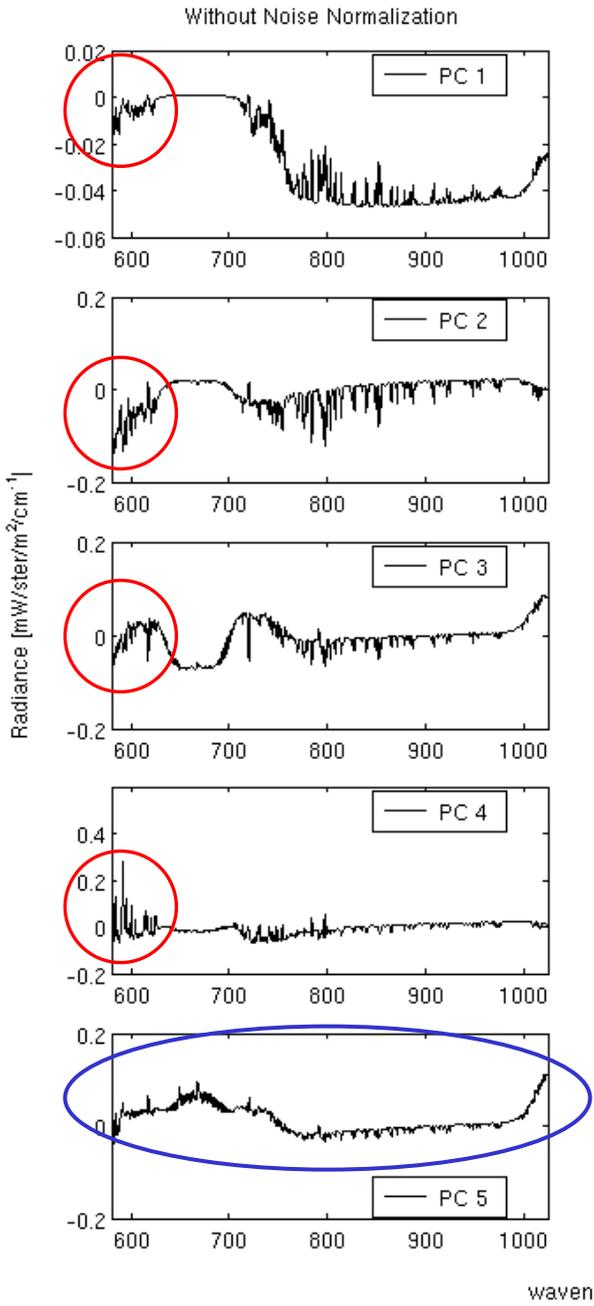
PNF approaches theoretical limits defined Linear Estimation Theory

# Importance of Noise Normalization

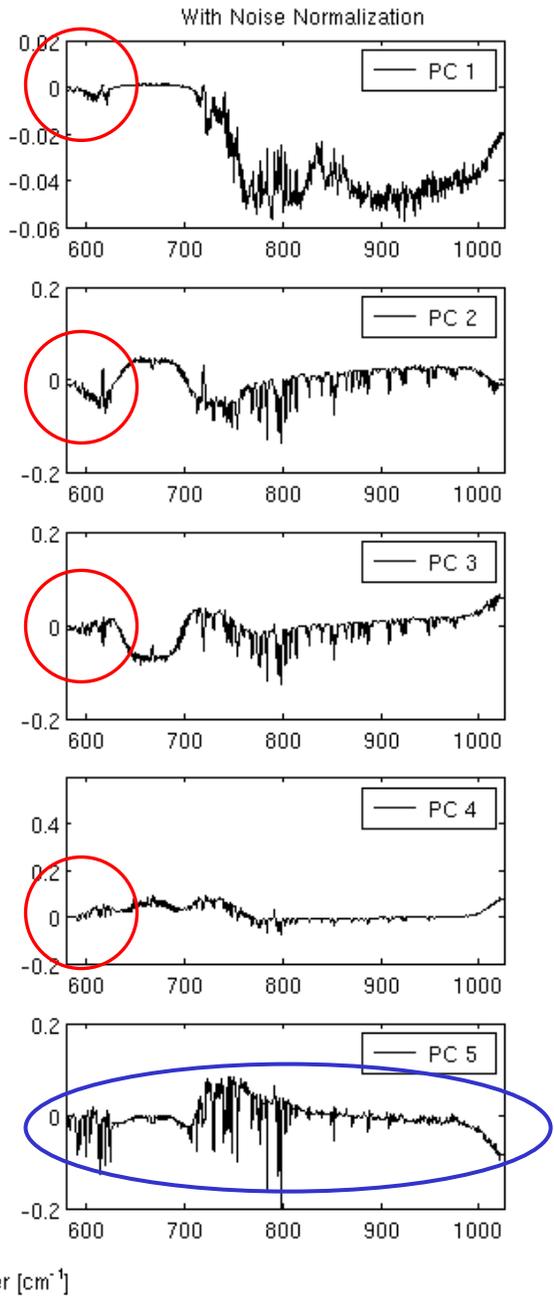


Noise Normalization changes noise distribution along different PCs

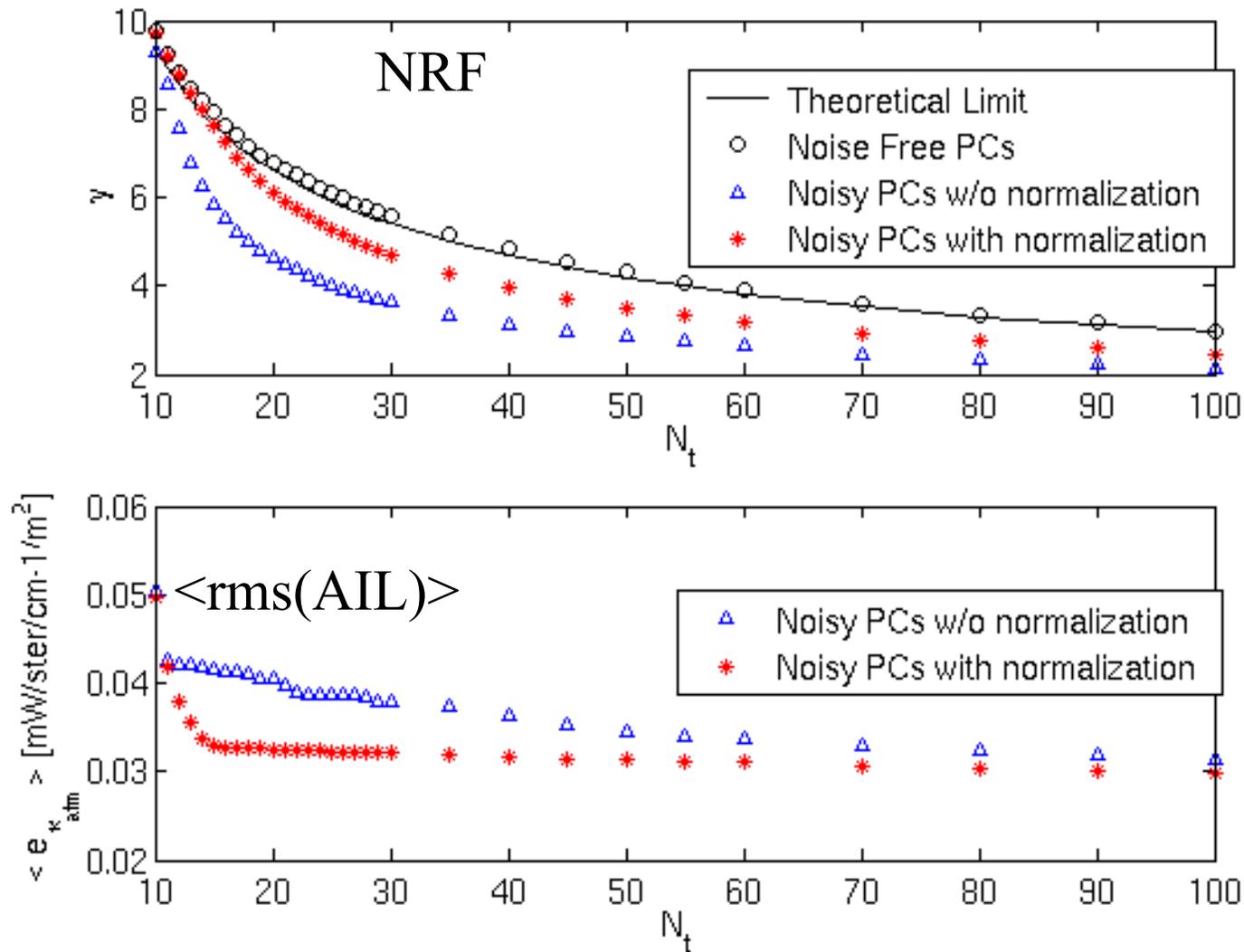
# PCs Without Noise Normalization



# PCs With Noise Normalization

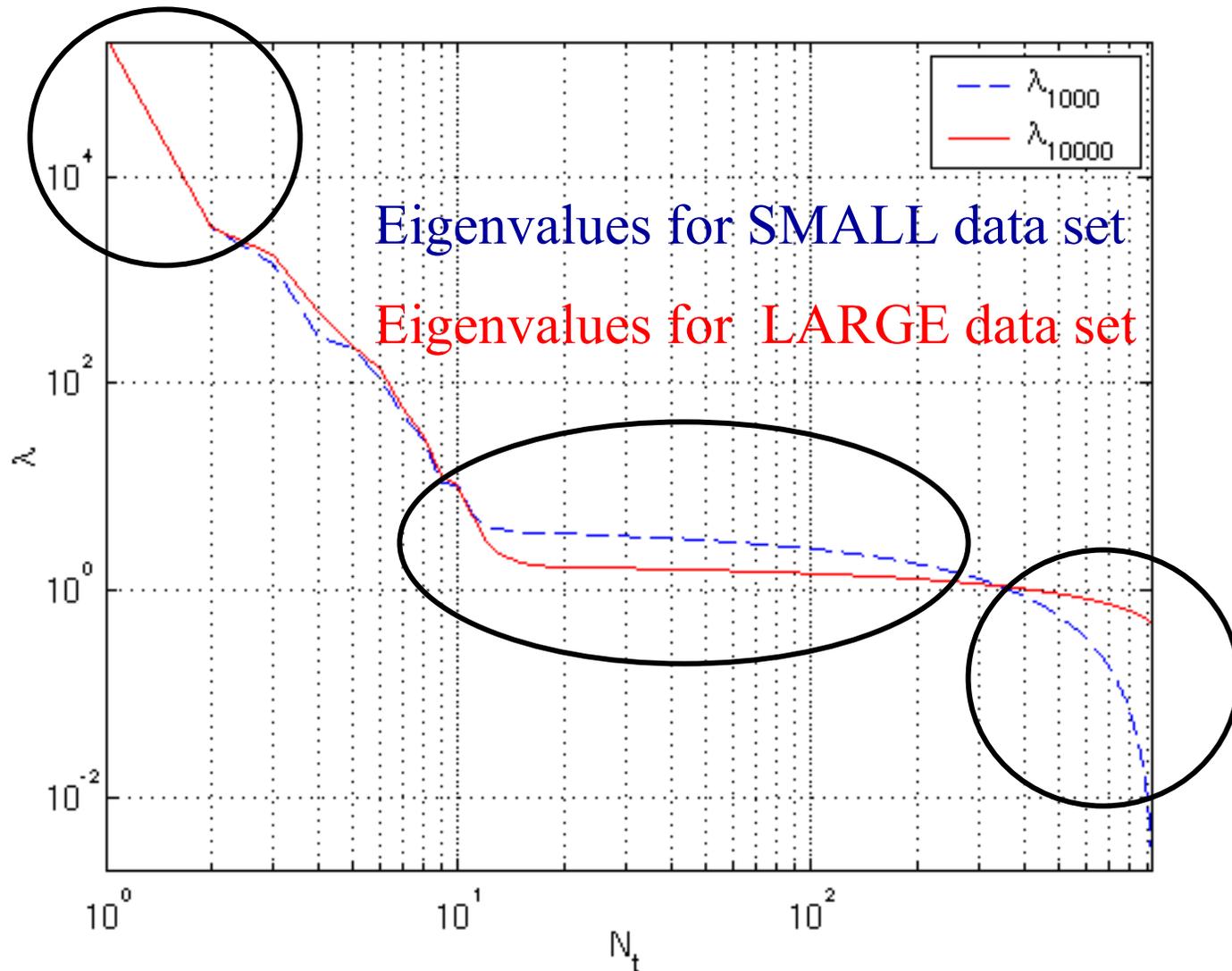


# Importance of Noise Normalization



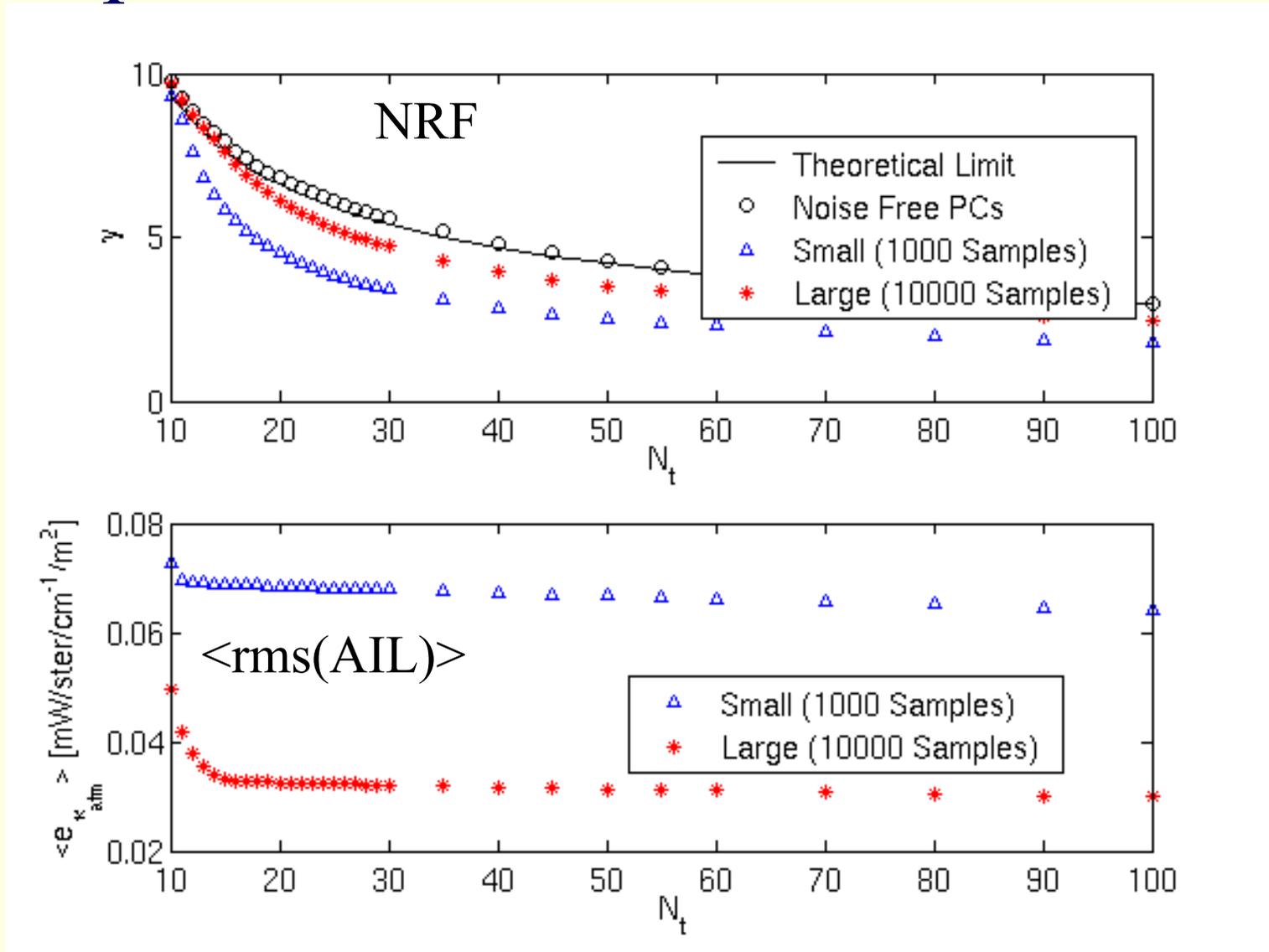
Noise Normalization increases NRF and decreases Atm. Info Loss

# Training Set Size



More Noise Variance explained by high order PCs (large values of  $N_t$ )

# Importance of Noise Normalization



Large Training Sets\* increase NRF and decrease Atm. Info Loss

# Conclusions on PNF impact on Simulated Data

- ◆ In RMS sense PNF approaches optimal values defined by Linear Estimation Theory for both AIL and RN
- ◆ RMS of AIL and RN are about 7 times\* smaller than RMS of Original Noise
- ◆ Noise normalization and Large Training Sets improve filter efficiency and accuracy

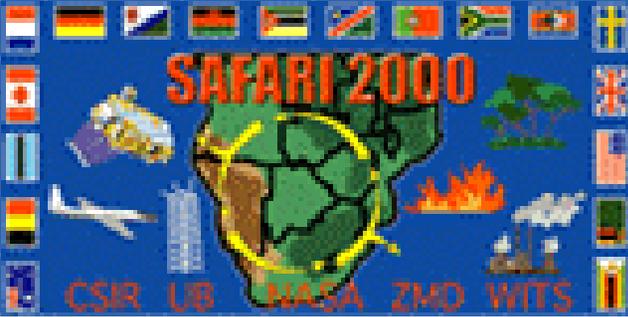
\* This Value depends on the specific instrument used



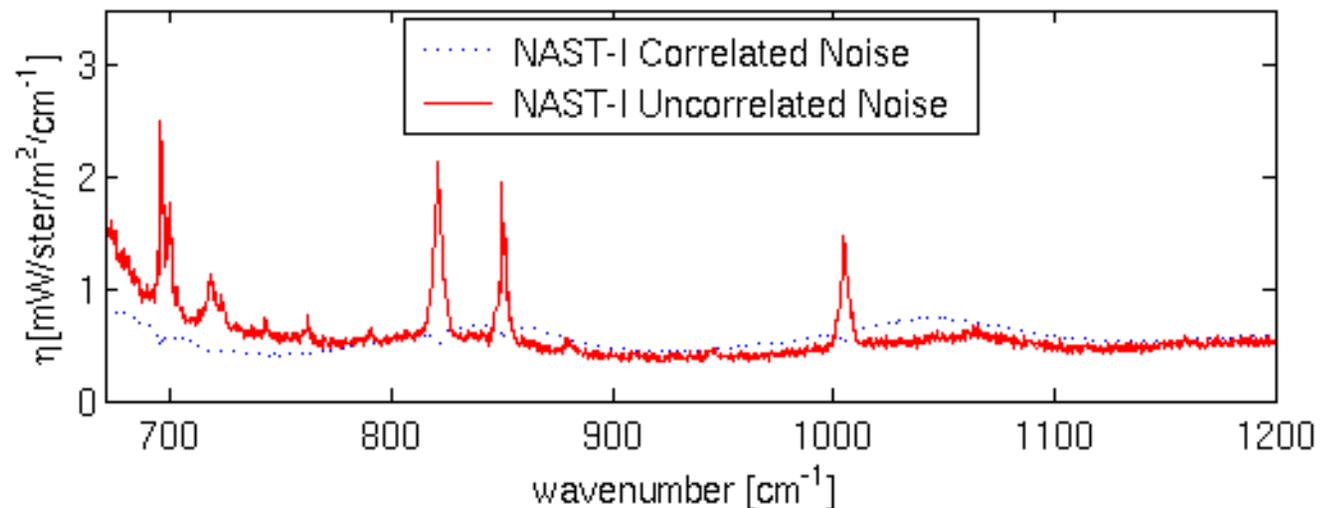
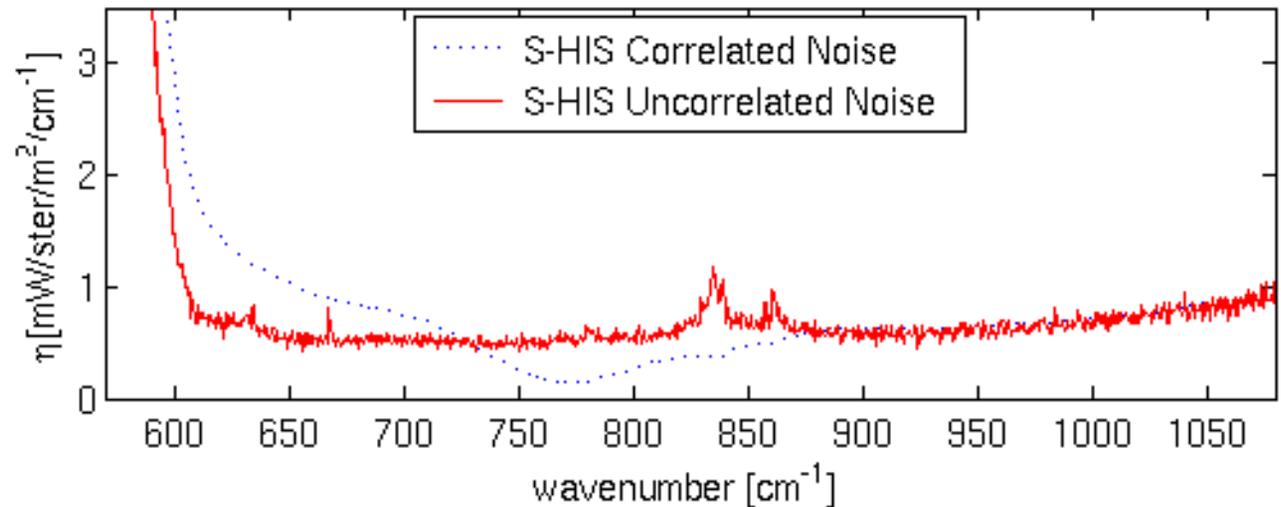
# Real Data: Platforms & Instruments



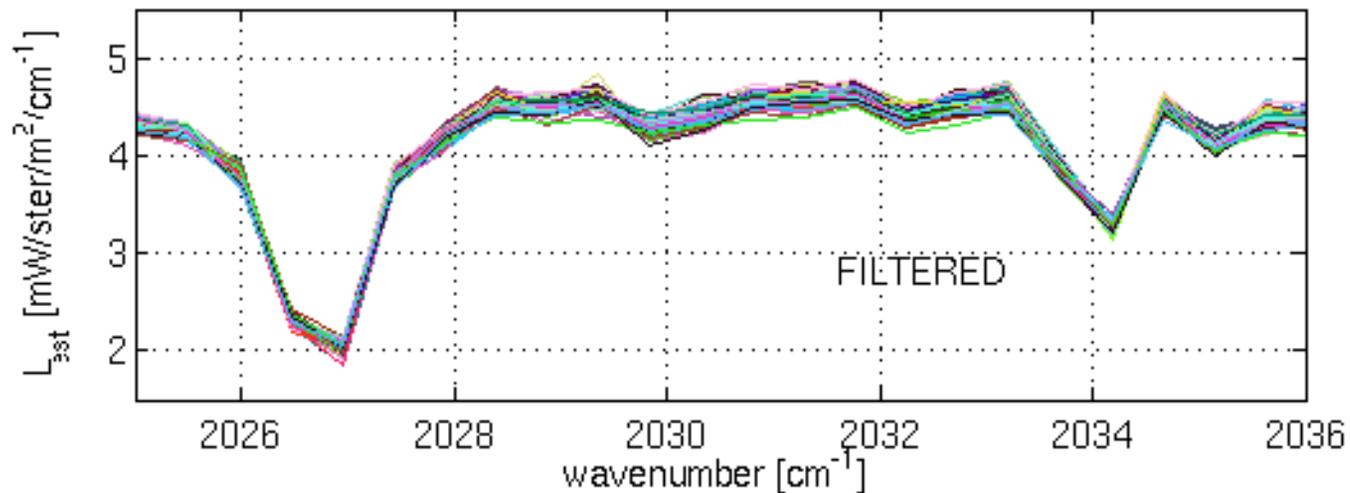
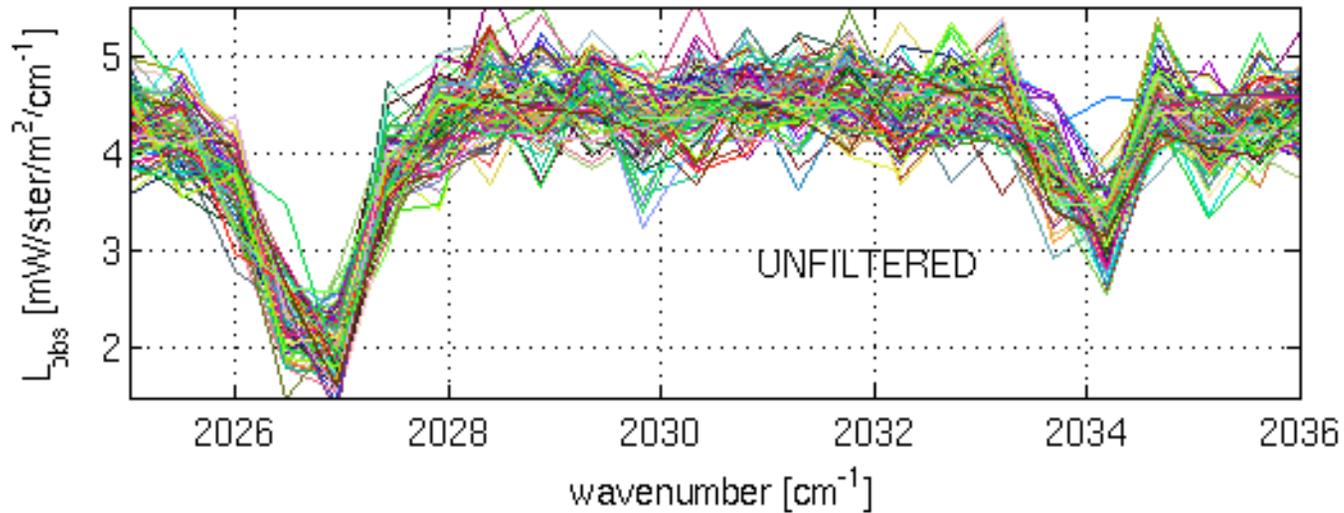
- ▶ ER-2 (cruise altitude: 20 km), its instruments are above 94% of the earth's atmosphere
  - NAST-I (FTS, 3.7-16 microns @ .25  $\text{cm}^{-1}$ )
  - S-HIS (FTS, 3.3-18 microns @ .5  $\text{cm}^{-1}$ )
  
- ▶ AQUA (Orbit altitude 705 km)
  - AIRS (Grating, 3.7-15.4 microns, resolving power 1200)



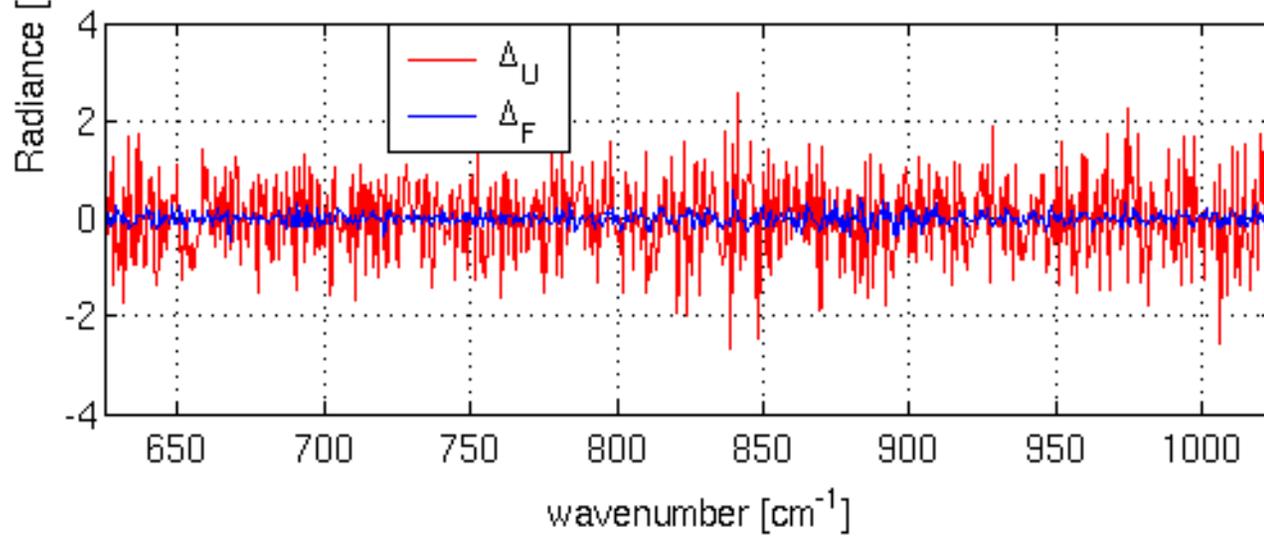
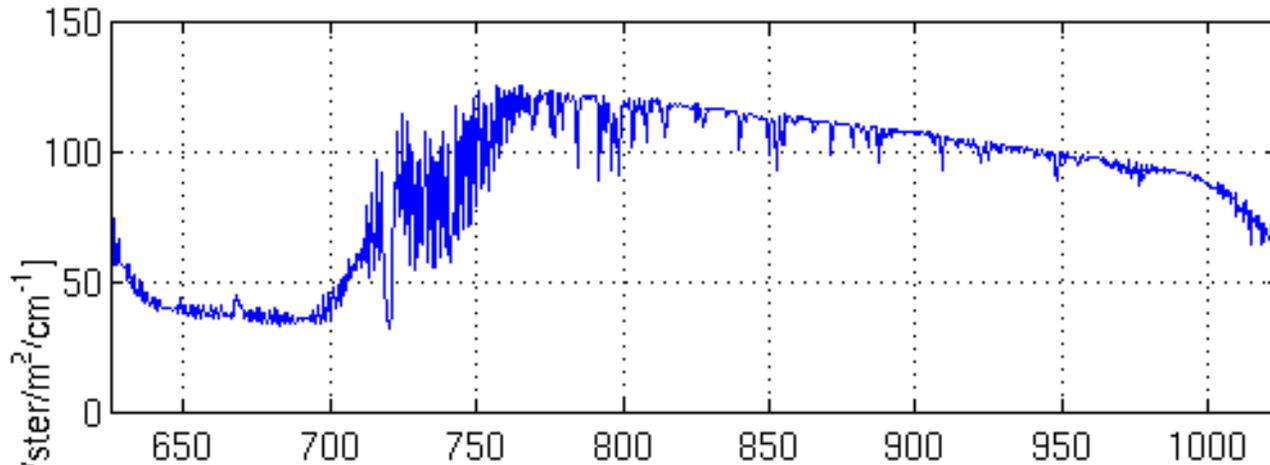
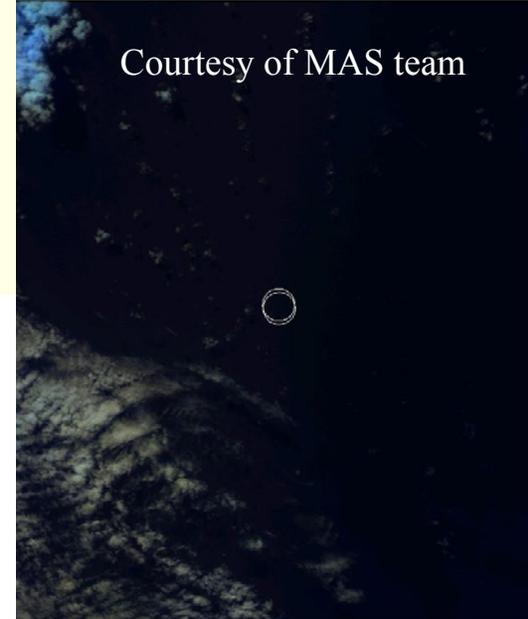
# Training Set: S-HIS from SAFARI 2000



# The Noise Filter Effect



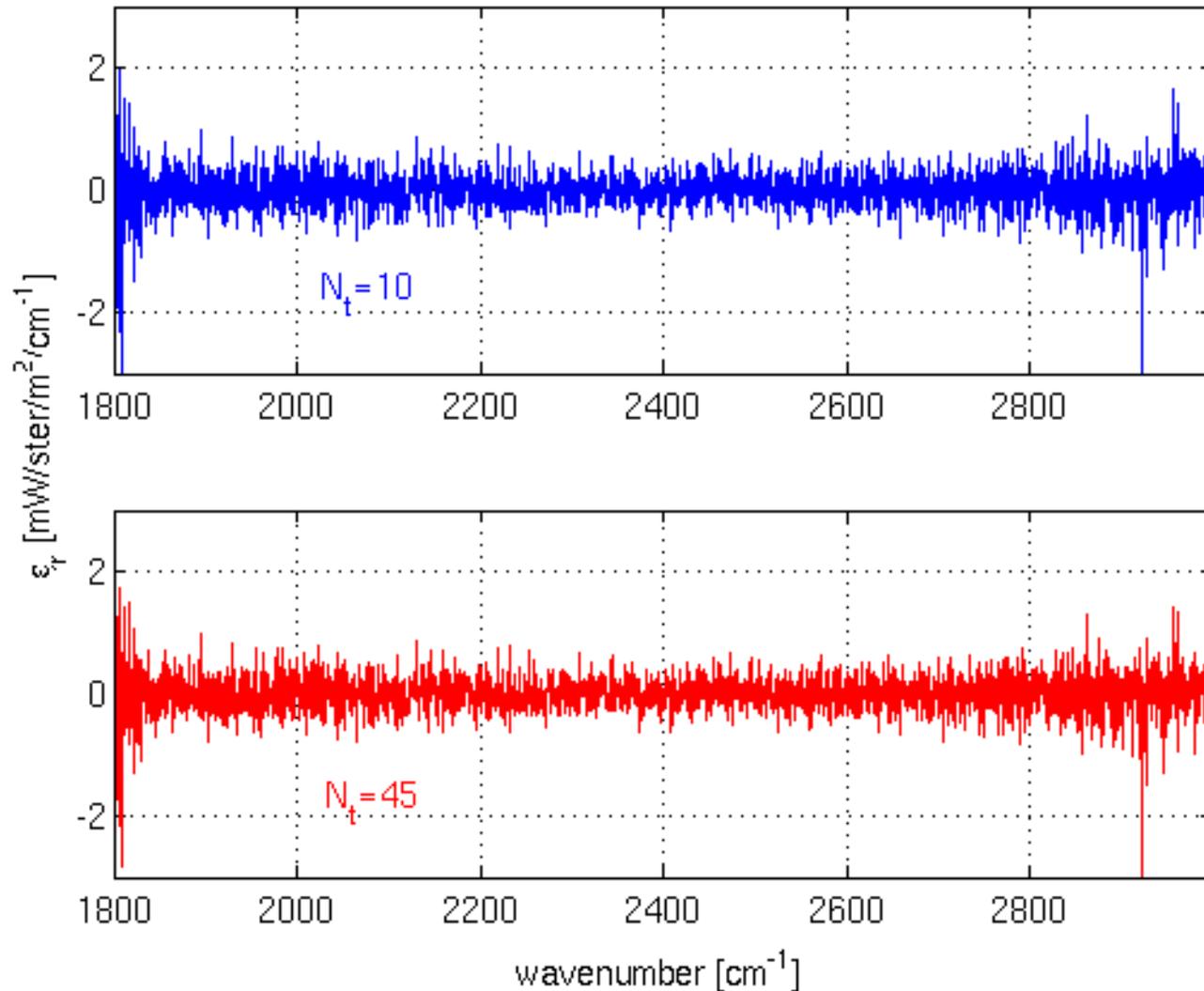
# Filtered-Unfiltered for almost overlapping FOVs over Ocean



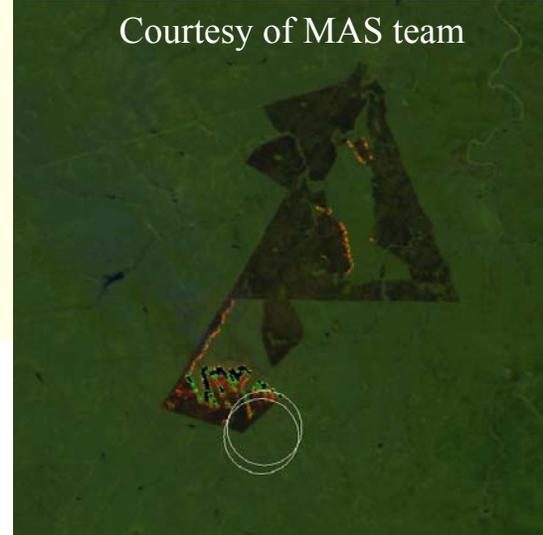
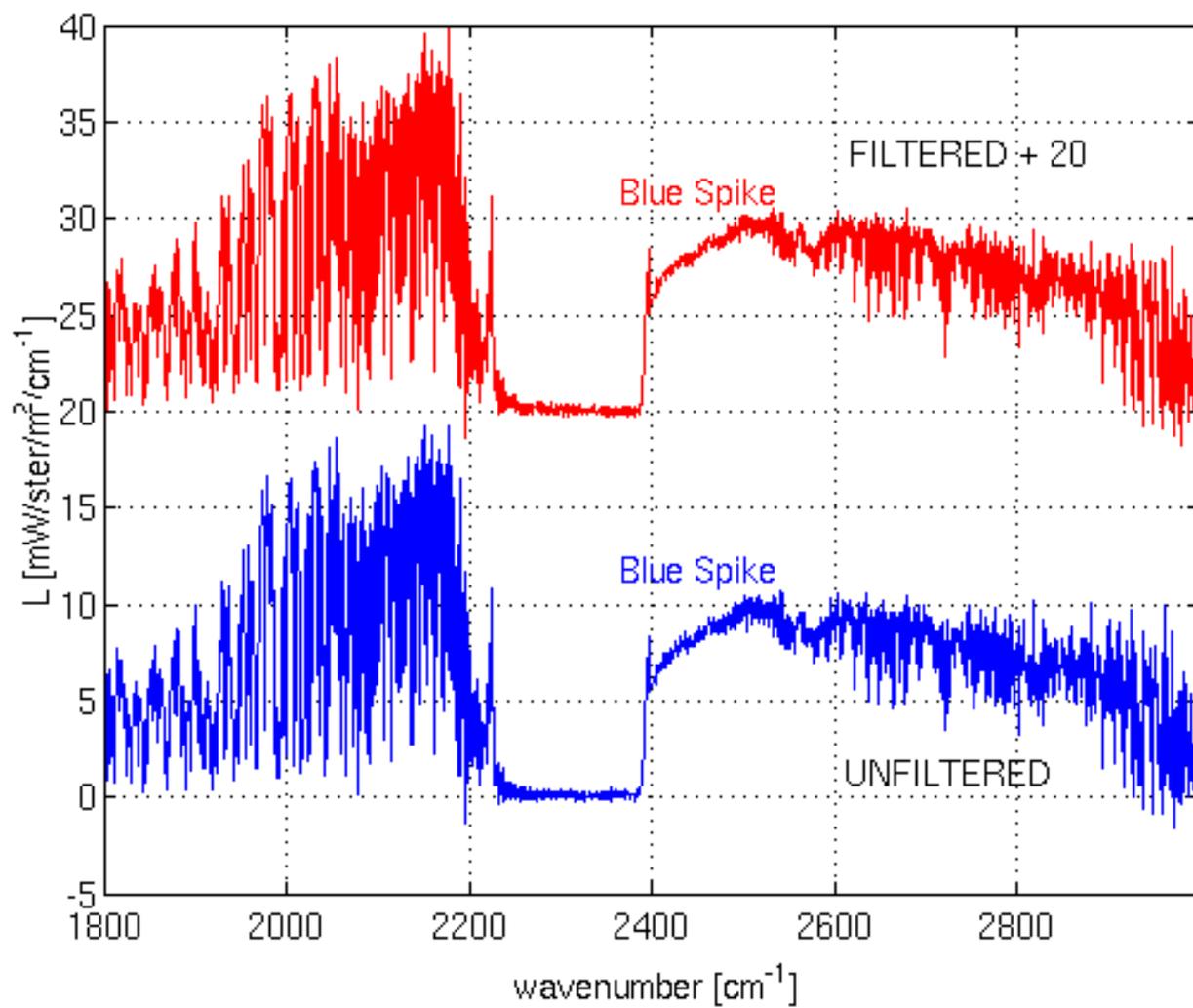
Unfiltered

Filtered

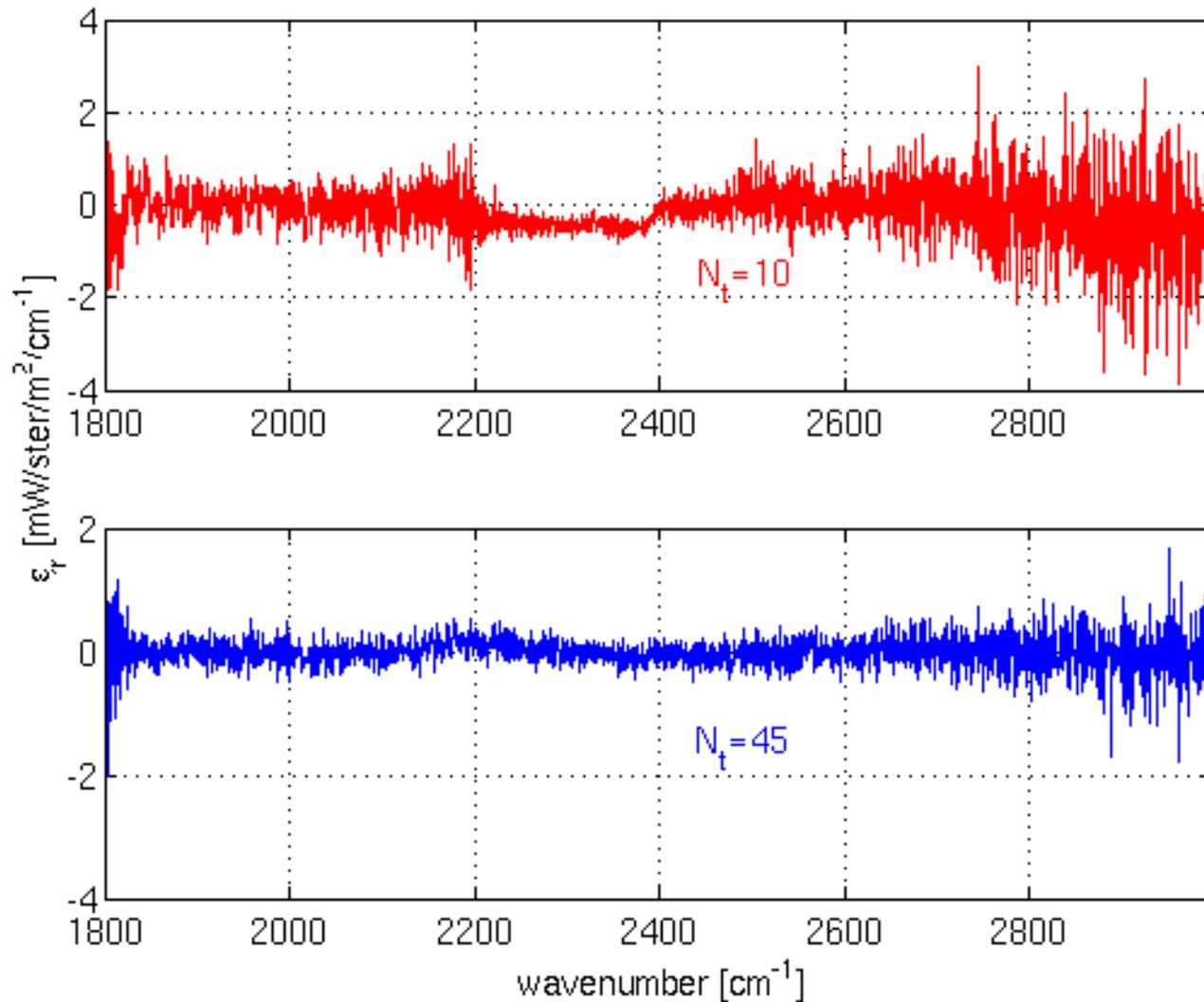
# Filtered-Unfiltered single FOV over Ocean

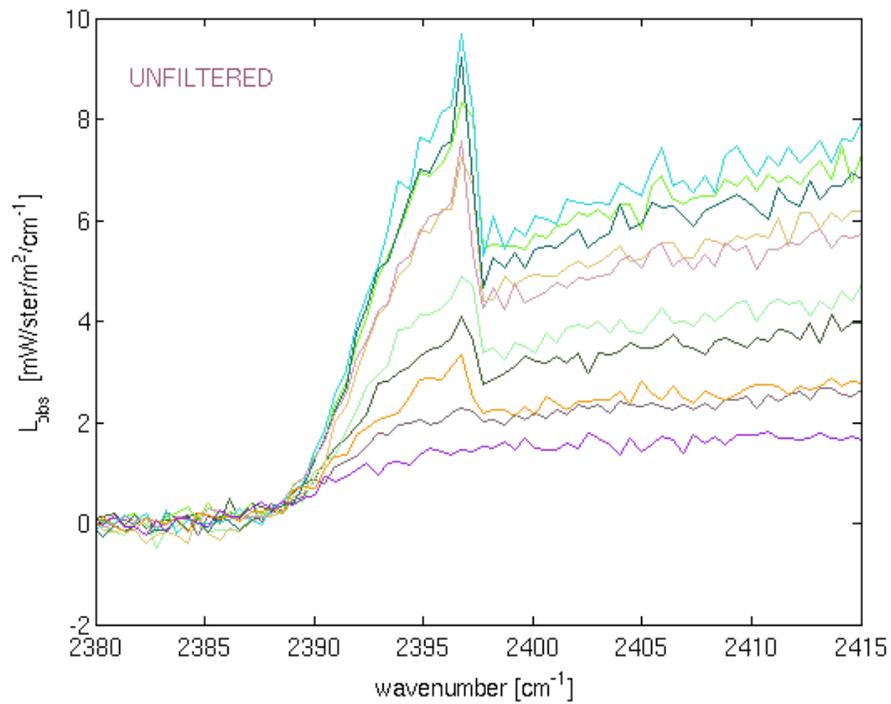


# Filtered and Unfiltered data for almost overlapping FOVs over Fire



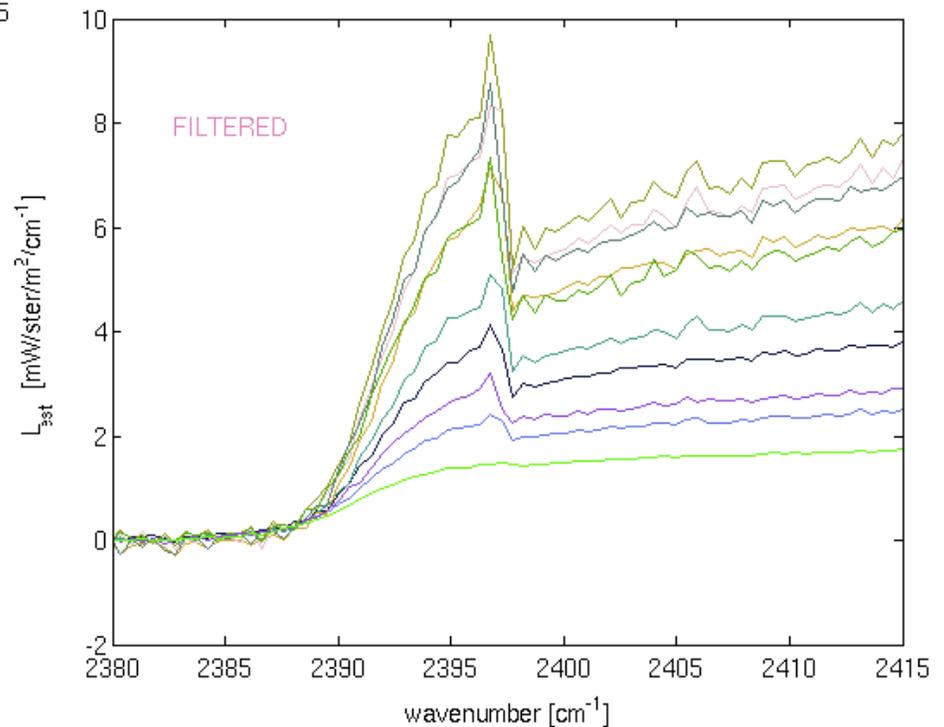
# Filtered-Unfiltered for almost overlapping FOVs over Fire

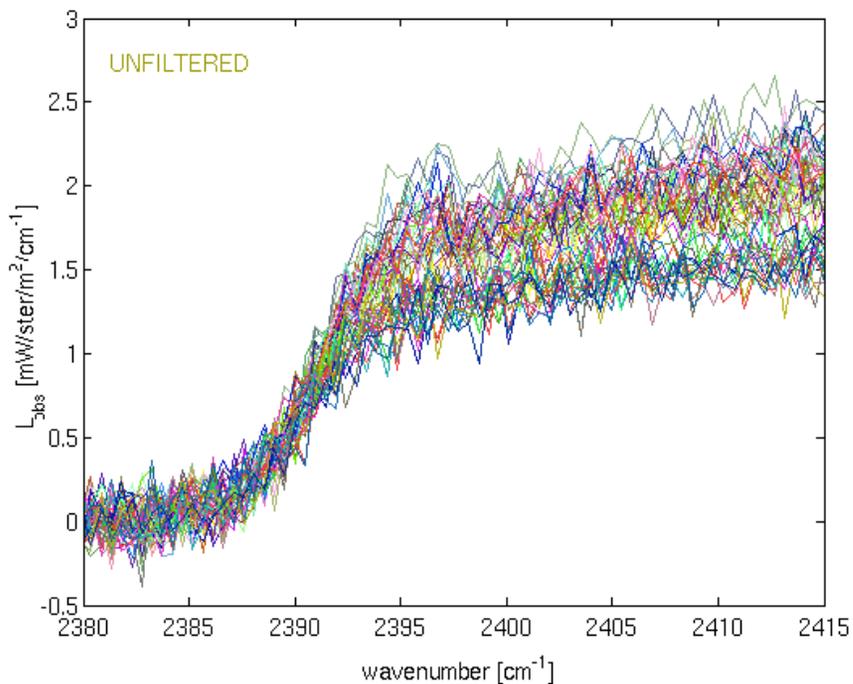




Unfiltered data for 10  
FOVs over Fire

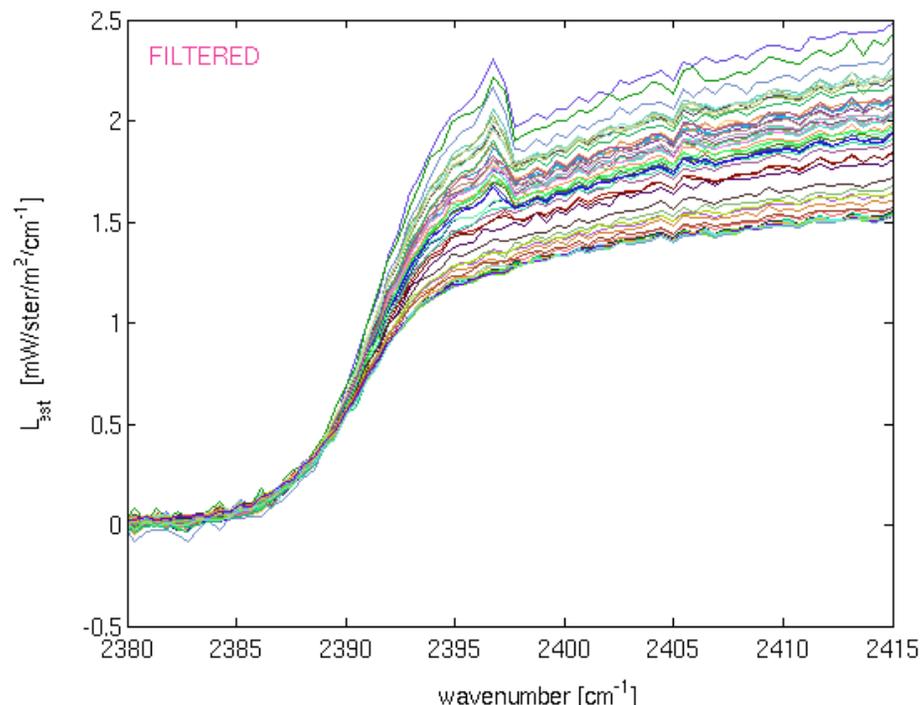
Filtered data for 10  
FOVs over Fire





Unfiltered data for 10  
FOVs after Fire

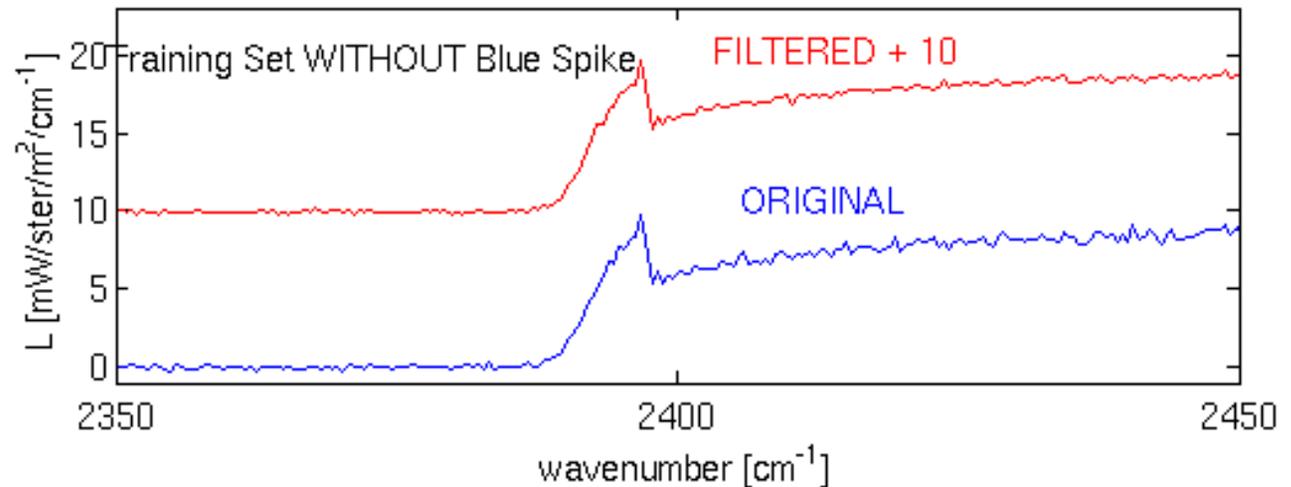
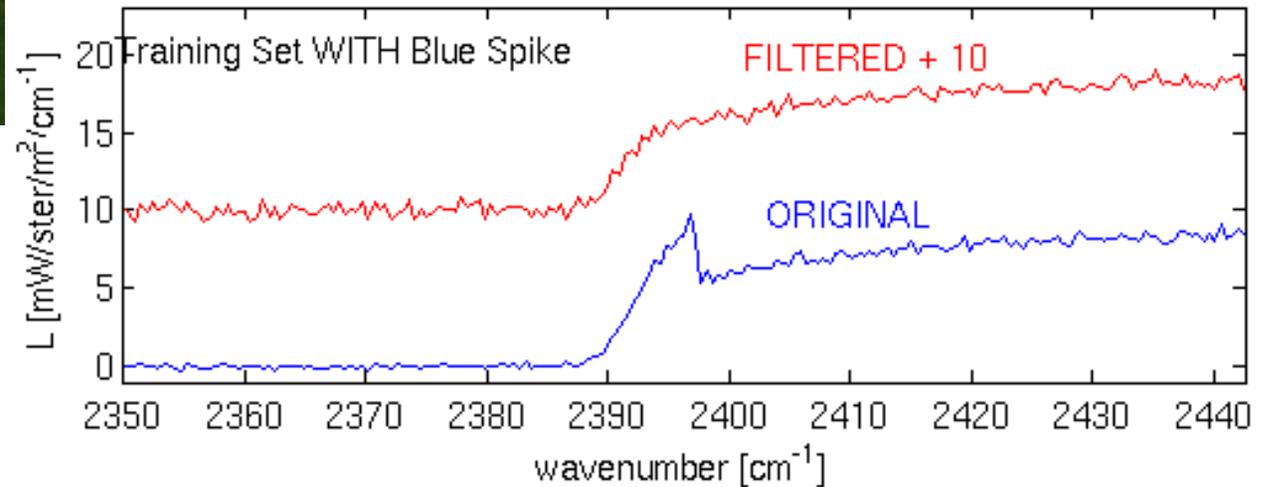
Filtered data for 10  
FOVs after Fire



# Importance Dependent Training

Poorly  
Estimated

Properly  
Estimated

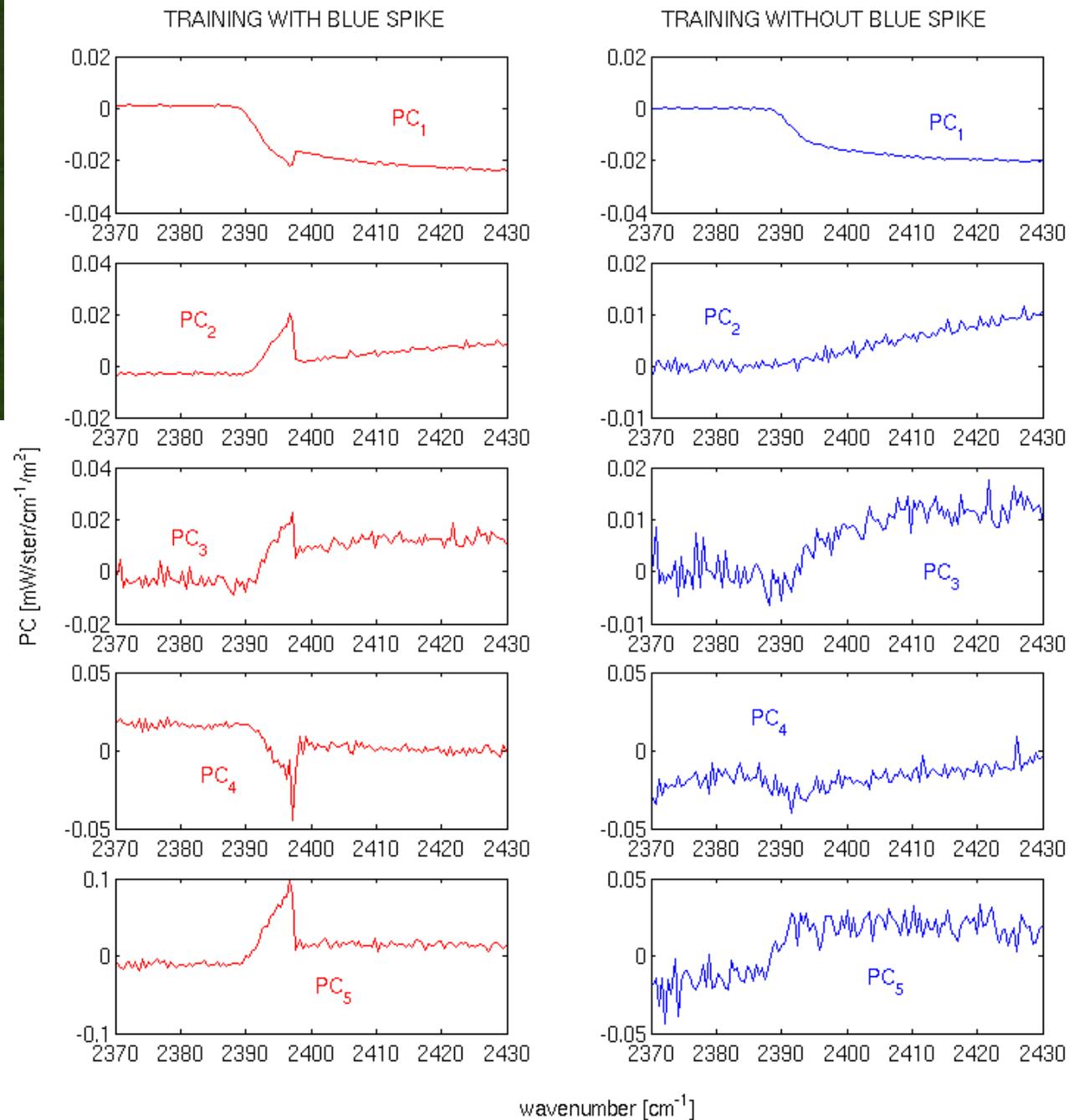


Courtesy of MAS team



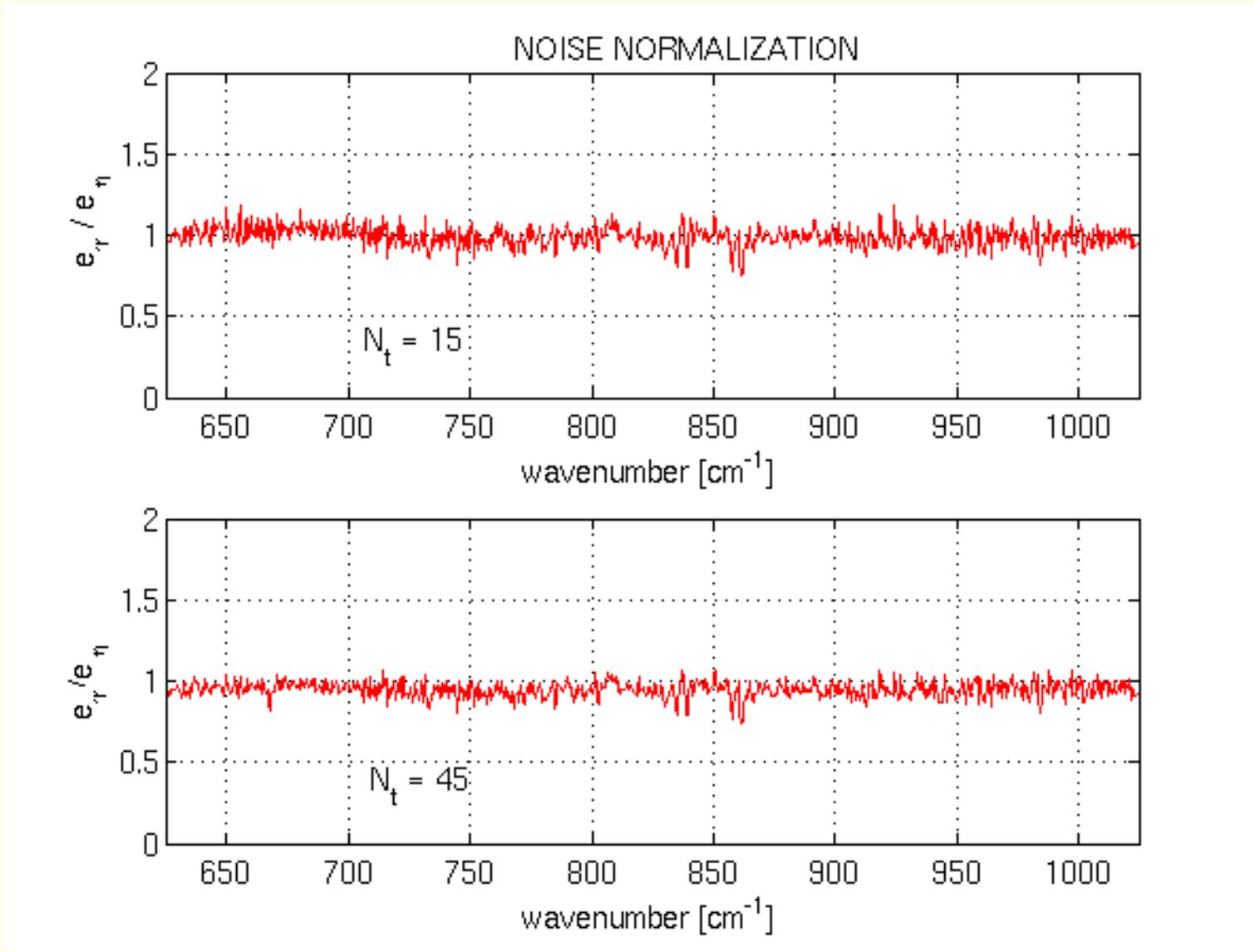
Training Set  
with  
Blue Spike

Training Set  
without  
Blue Spike



wavenumber [cm<sup>-1</sup>]

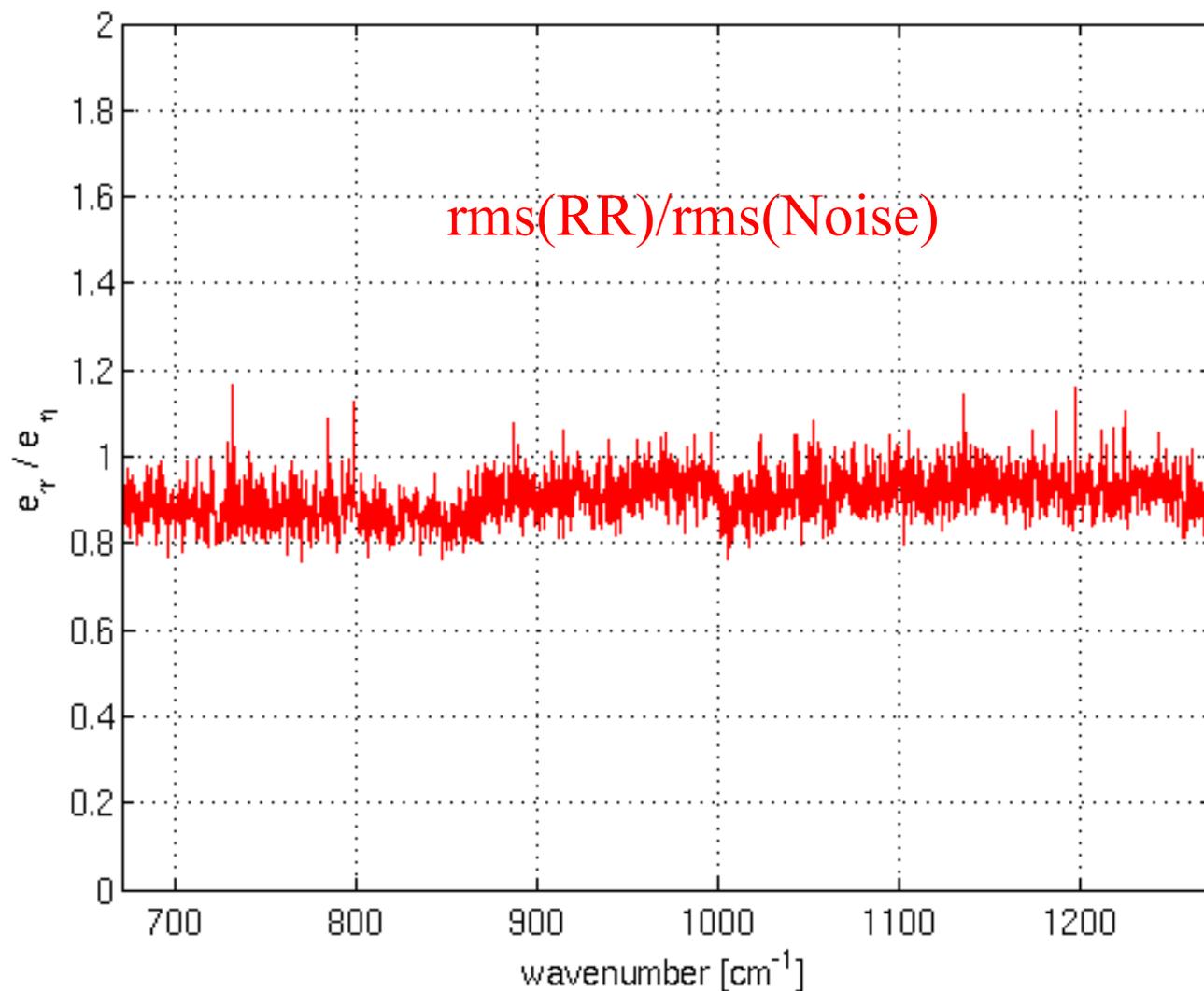
# Importance of Noise Normalization



$\text{rms}(\text{RR}) / \text{rms}(\text{Noise})$

Noise normalization avoids fitting noise where noise level is high

# PNF used for noise estimation

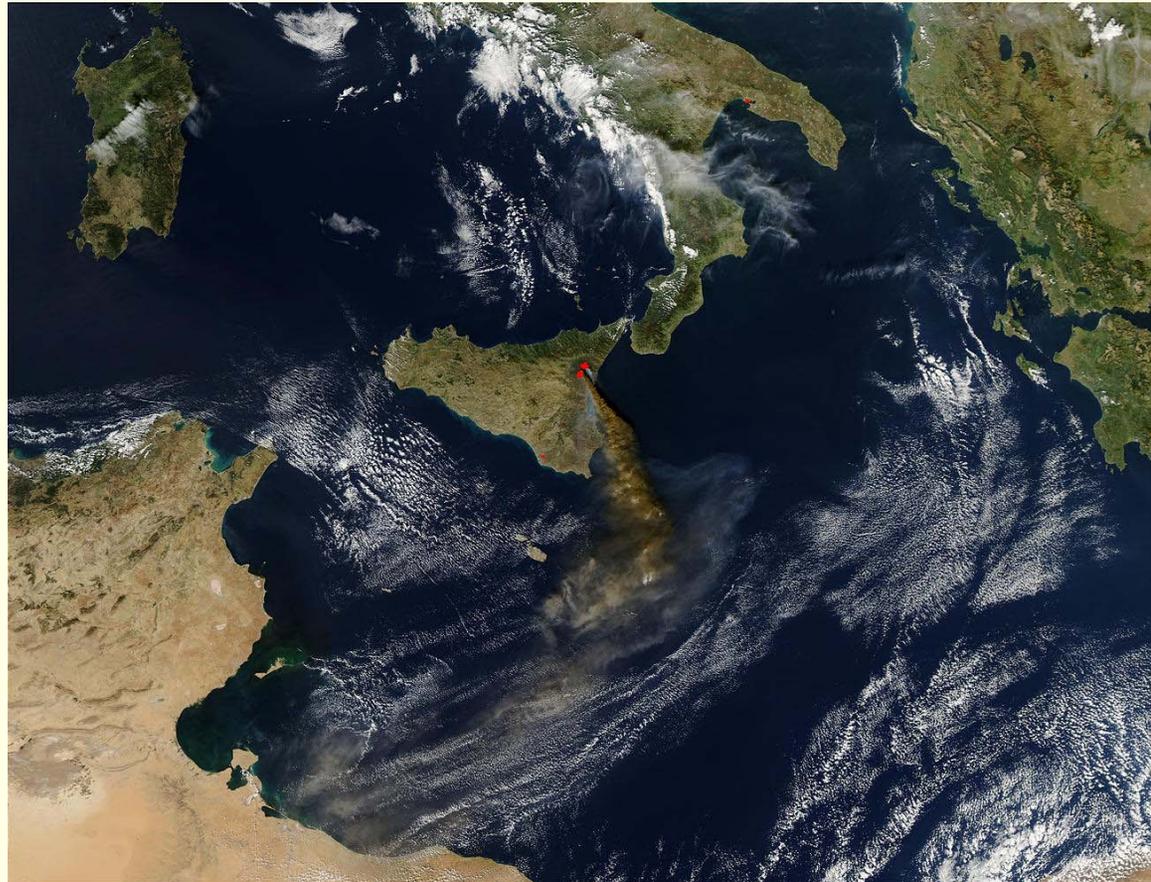
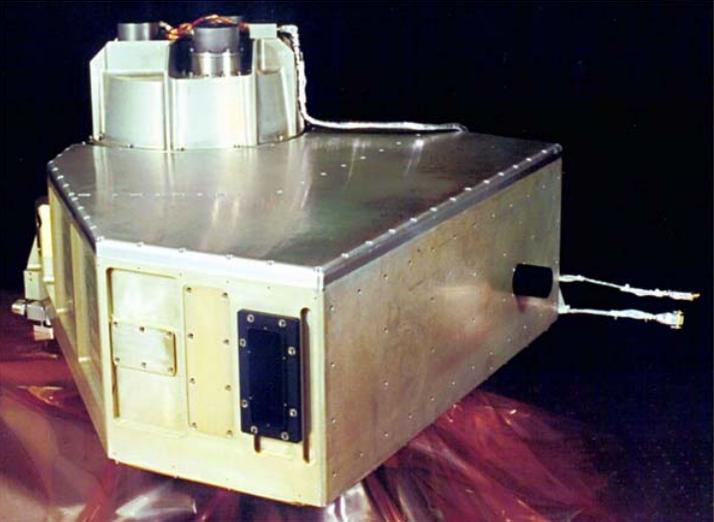


$\langle \text{rms}(\text{RR}) \rangle$

$\partial \langle \text{rms}(\text{RR}) \rangle / \partial N_t$

Noise estimation with PNF still not objective!

# AIRS on Mount Etna



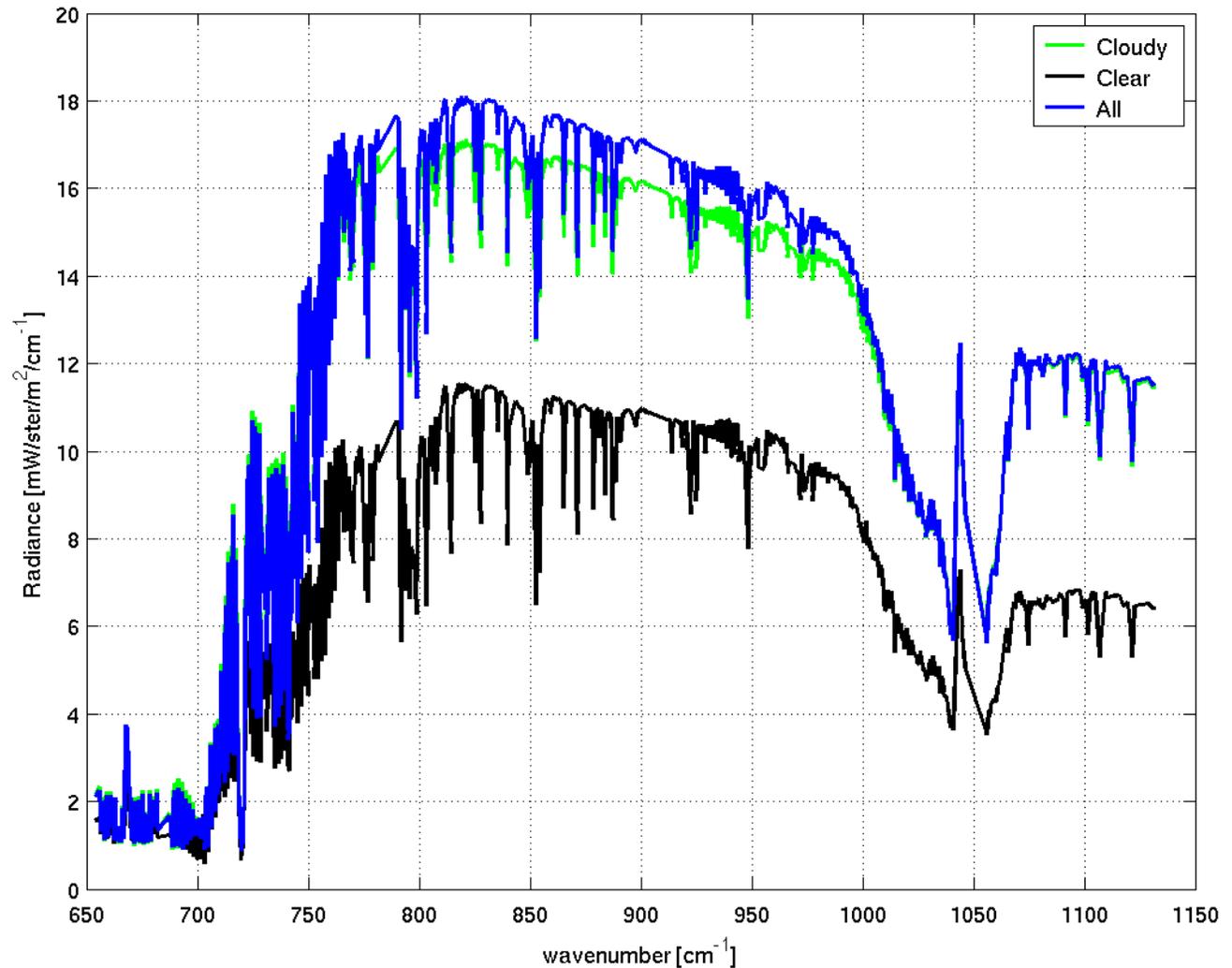
# Signal Variance

## Granule 123, 28 Oct 2002

Cloudy

Clear

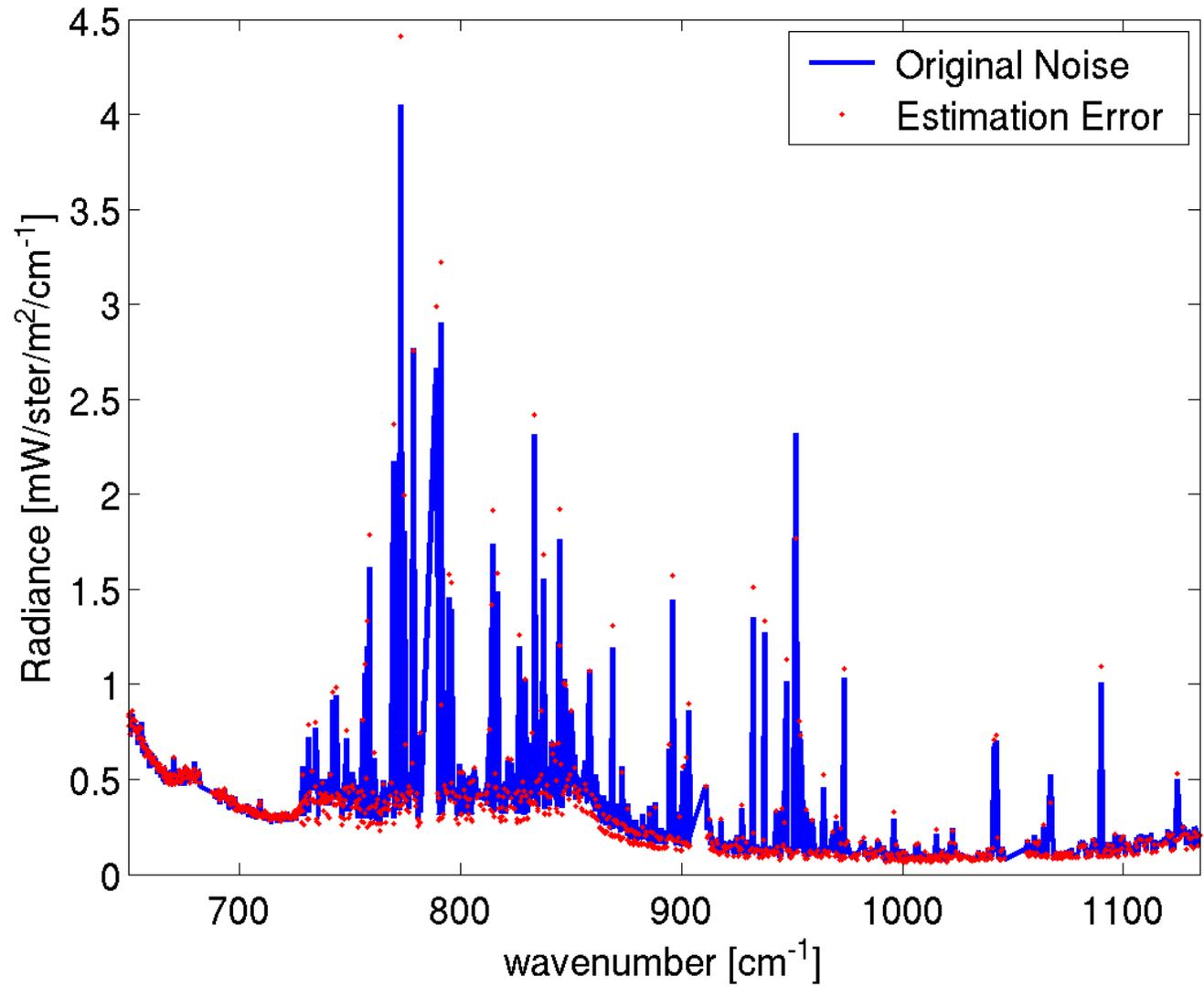
All



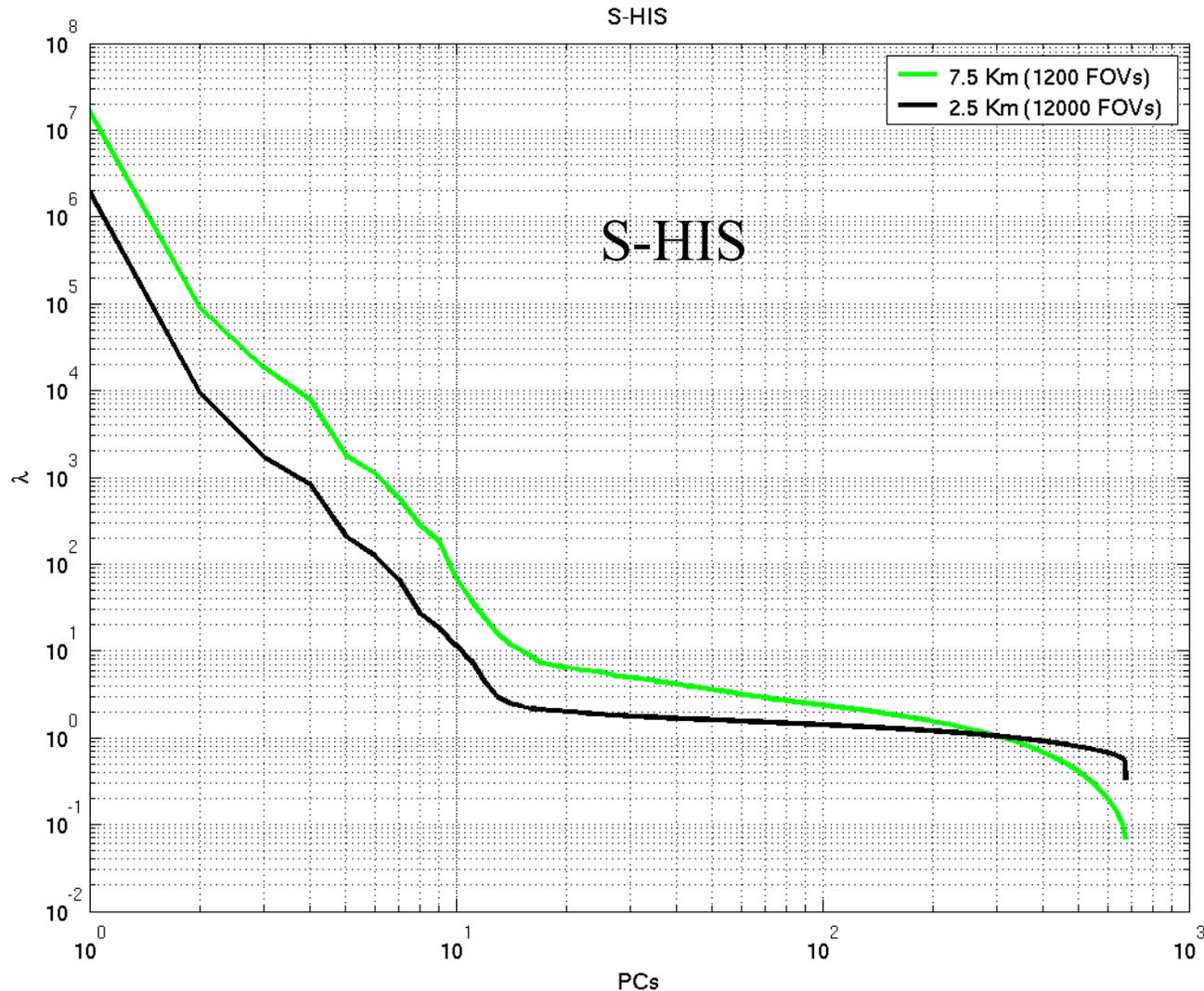
# AIRS noise

From Granule

Estimated  
Noise

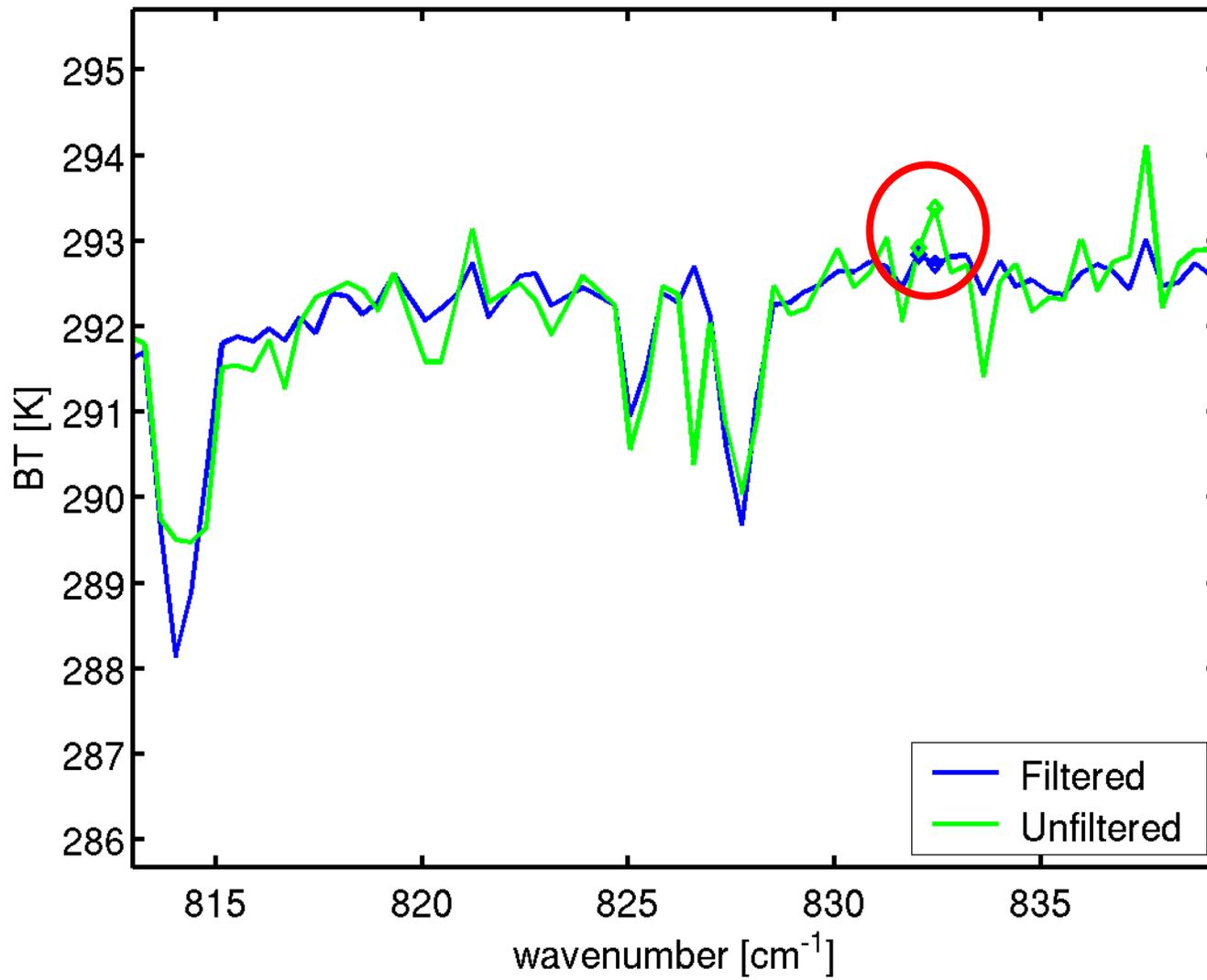


# Eigenvalues of Obs covariance Matrix

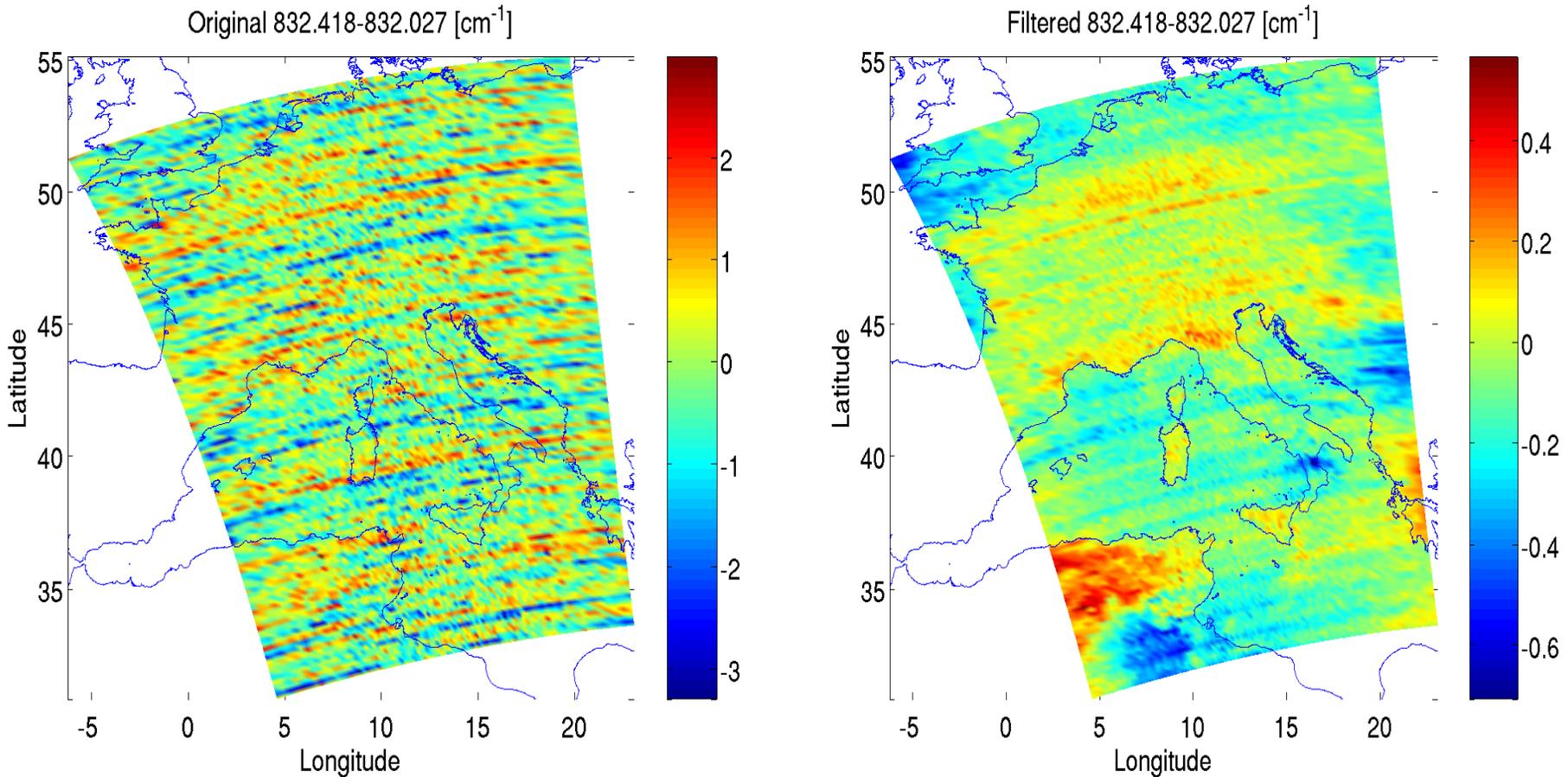


Larger Training with more redundant observation == Smaller FOVs

# AIRS channel differences

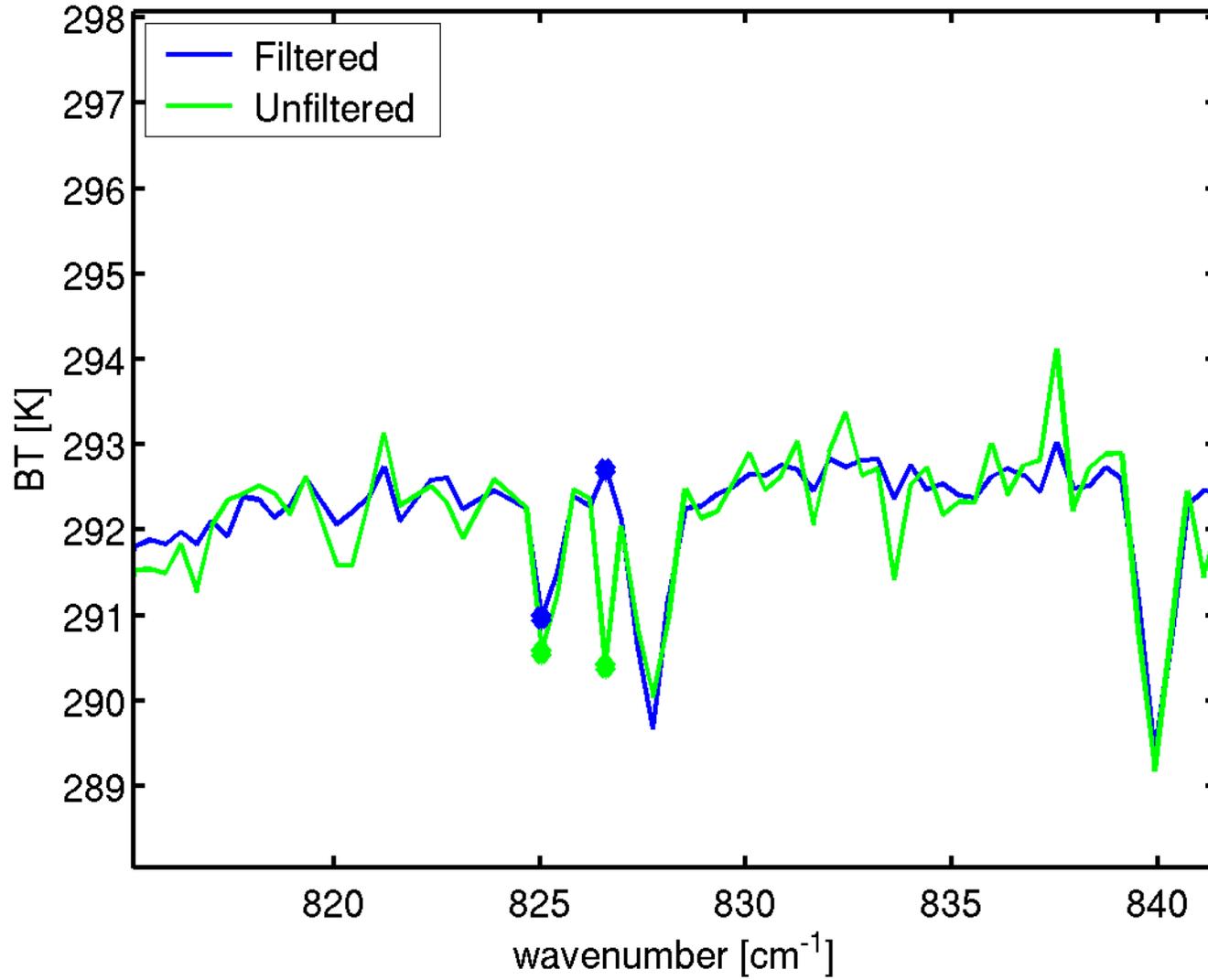


# Filter vs Unfiltered

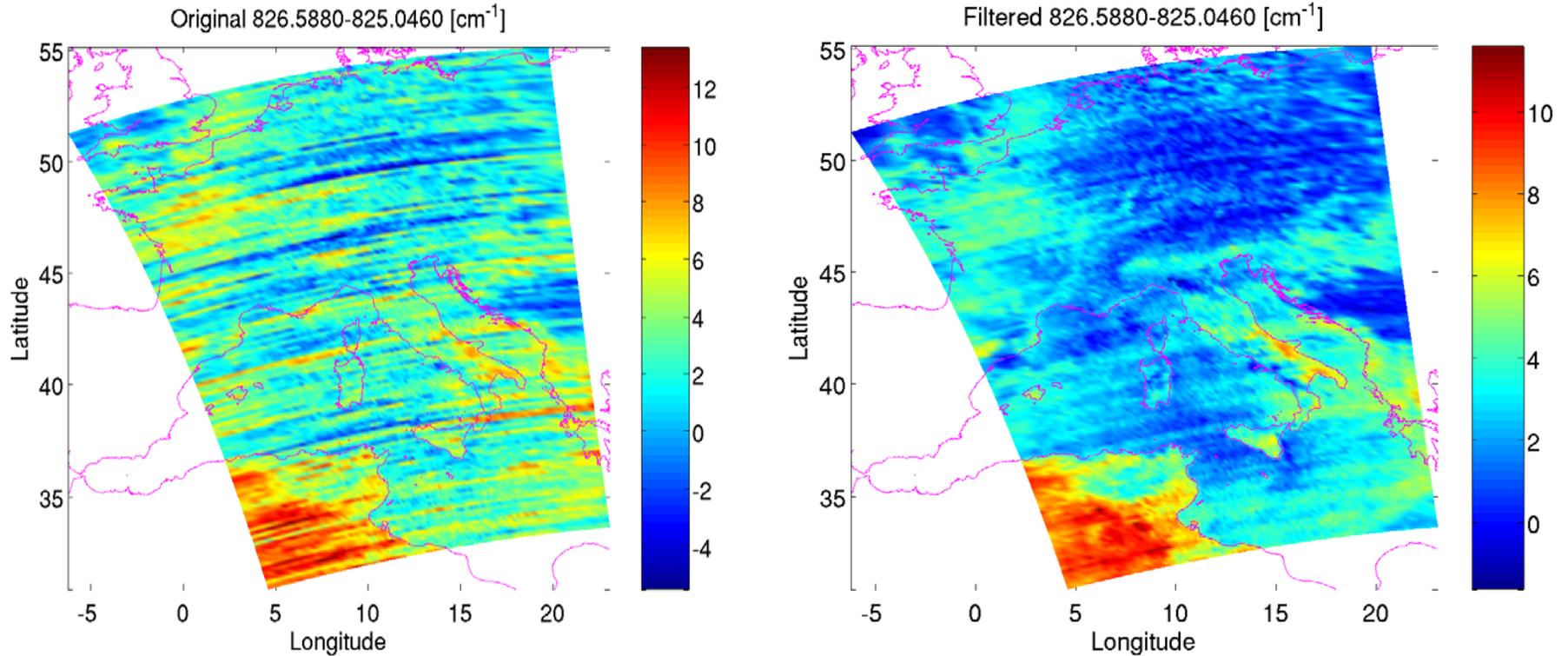


Features over Northern Africa and Southern Italy are visible after filtering

# AIRS channel differences

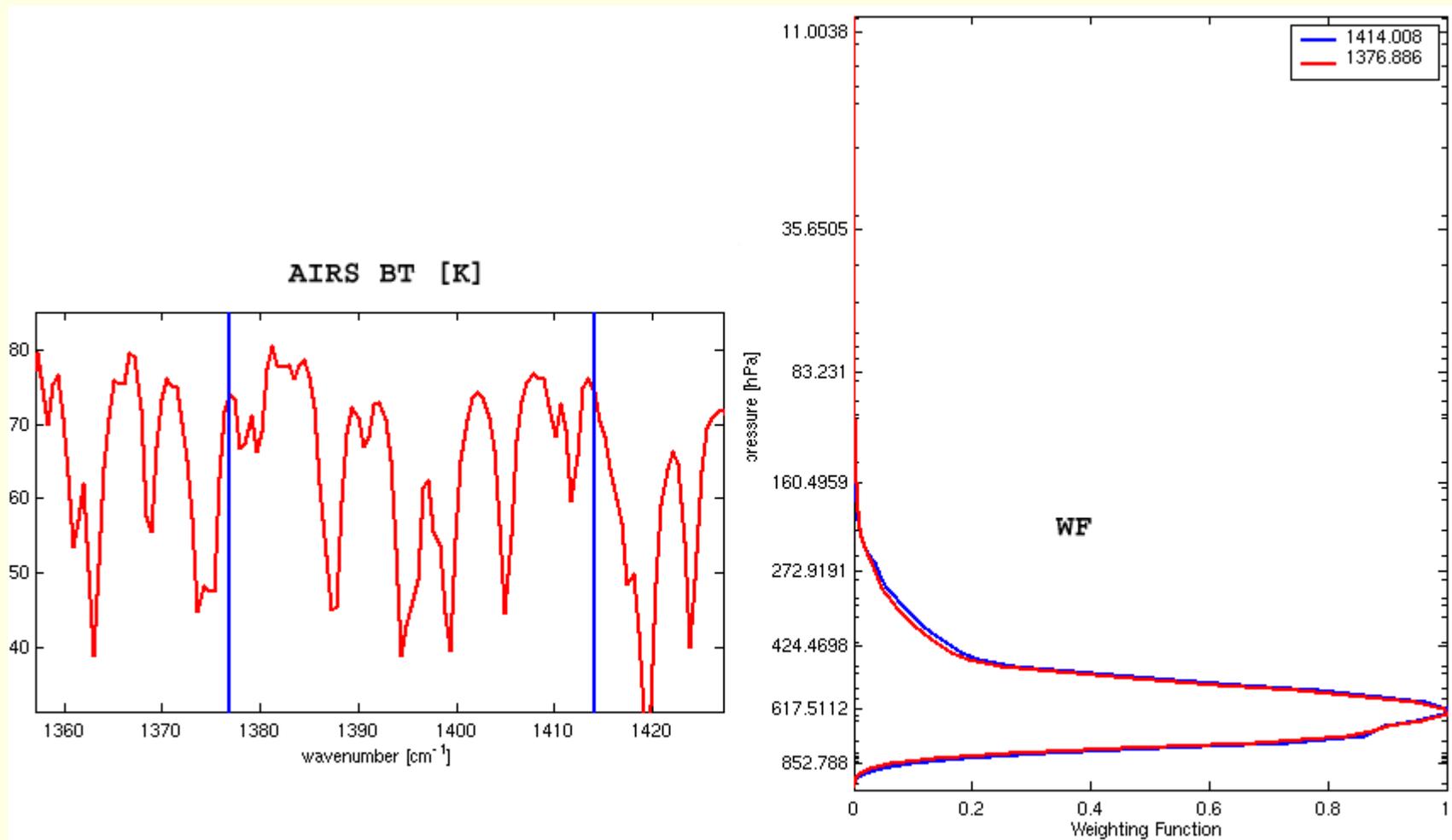


# Filter vs Unfiltered



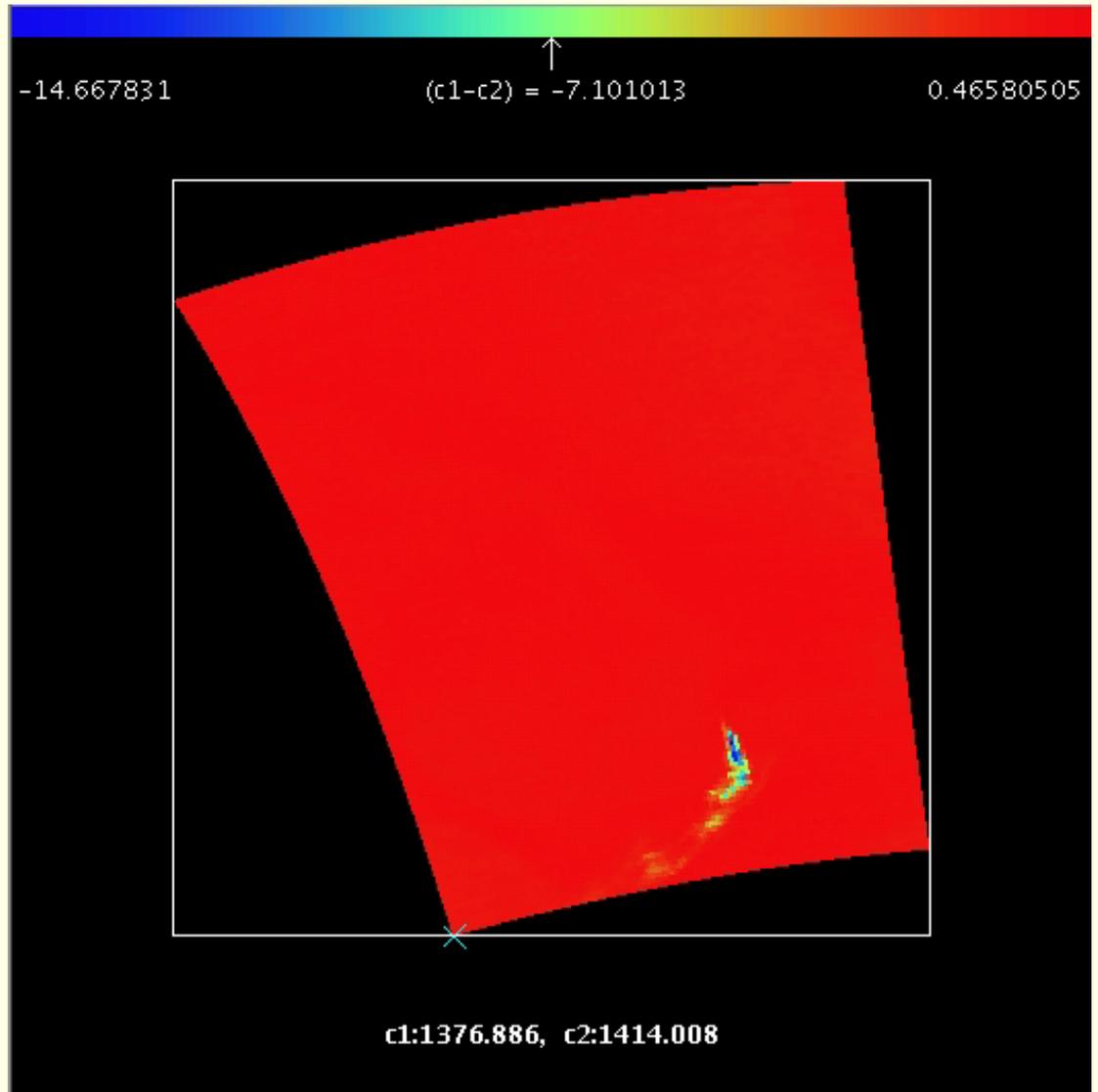
Striping is removed and features over Northern Africa are visible after filtering

# Sensitivity to SO<sub>2</sub>



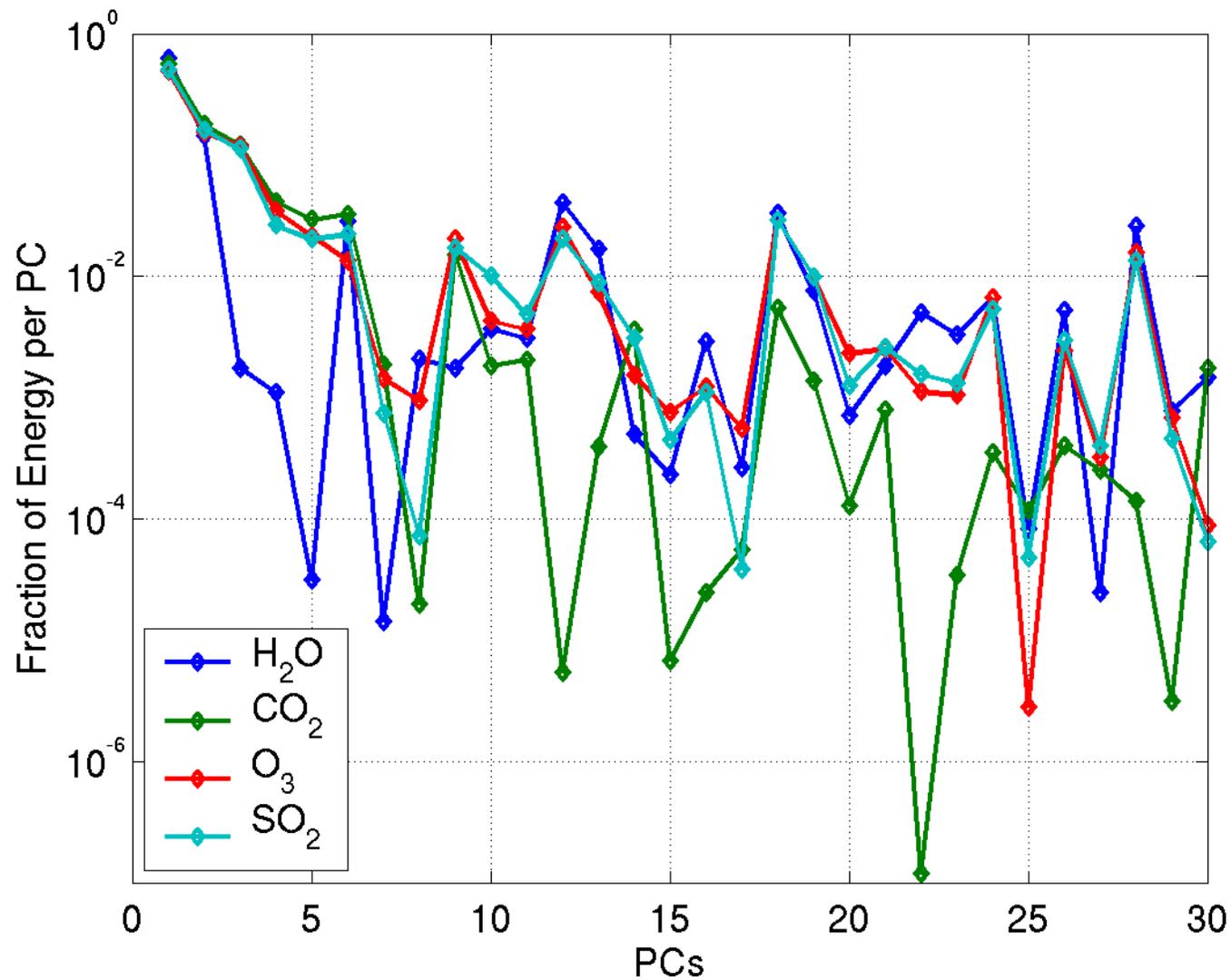
Work initiated by  
Larrabee Straw  
And Dave Tobin

# SO<sub>2</sub> emitted by Mount Etna



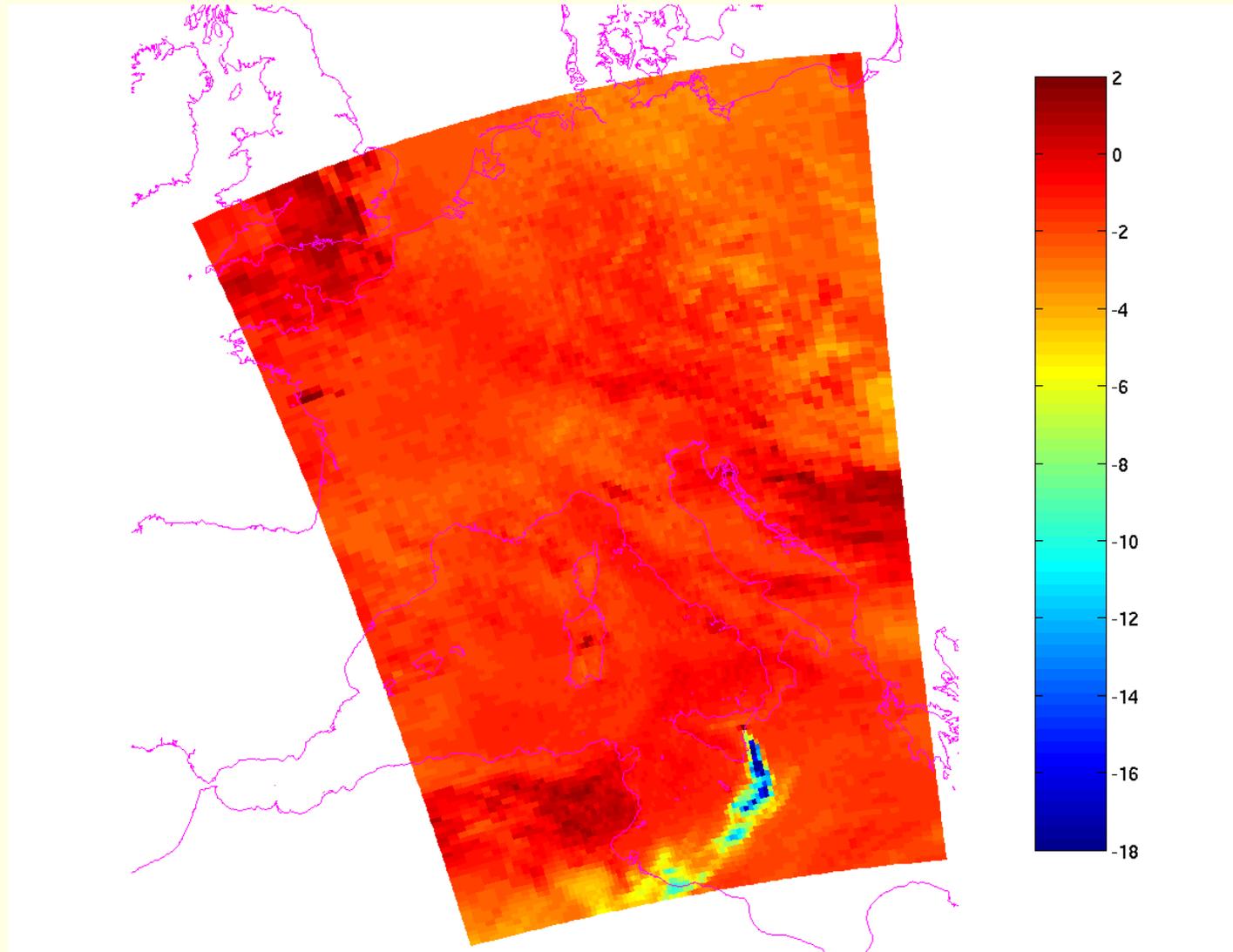
1414.008-1376.886 cm<sup>-1</sup>

# Fraction of Energy per PCs



# SO<sub>2</sub> Concentration

PCC8-PCC11



# Conclusions

- PCA by taking advantage of redundancy reduces random component of Instrument noise (PNF)
- Both AIL and RN approach the optimal value defined by Linear Estimation Theory
- For simulated data (presented case) AIL and RN are 7 times smaller than original noise
- Both AIL and RN are correlated in wavenumber space
- Most difficult cases, observation highly deviant from mean, are properly treated if PCs are derived in Dependent Mode

# Conclusions

- Noise normalization and large training set enhance accuracy and efficiency of PNF
- If not available, estimate of random component of instrument noise can be obtained by applying PCA to observations
- With real data (AIRS) achieved NR factor is between 4 and 5
- PNF is not quite ready to be used as Black Box, it requires tuning and monitoring of Reconstruction Residuals

## Ongoing Work

- Characterization of AIL and RN spectral correlation
- Investigation of physical meaning of PCs

**Thanks!**

**Questions?**