Optimization of NPOESS CrIMSS EDR Algorithm

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CrIMSS Overview

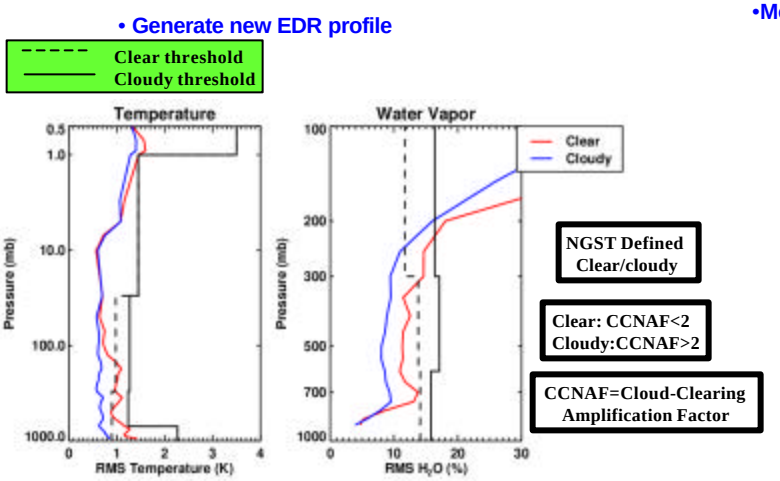
- Cross-track Infrared and Microwave Sounder Suite (CrIMSS)
  - •Consists of both infrared and microwave instruments for global atmospheric soundings
  - •Required Environmental Data Records (EDR)
    - •Temperature/water vapor/pressure profiles
  - •Infrared: Cross Track Infrared Sounder (CrIS)
    - •Band1: 650 cm^{-1} – 1095 cm^{-1} @ 0.625 cm^{-1}
    - •Band2: 1210 cm^{-1} – 1750 cm^{-1} @ 1.25 cm^{-1}
    - •Band3: 2155 cm^{-1} – 2550 cm^{-1} @ 2.5 cm^{-1}
  - •Microwave: Advanced Technology Microwave Sounder (ATMS)
    - •22 channels:
    - •Window channels: 23.8 GHz, 31.4 GHz, 88.2 GHZ, 165.5 GHz
    - •Temperature sounding: 13 channels 50-60 GHz
    - • Water vapor sounding channels: 5 in the183 GHz region

Optimization of CrIMSS Code

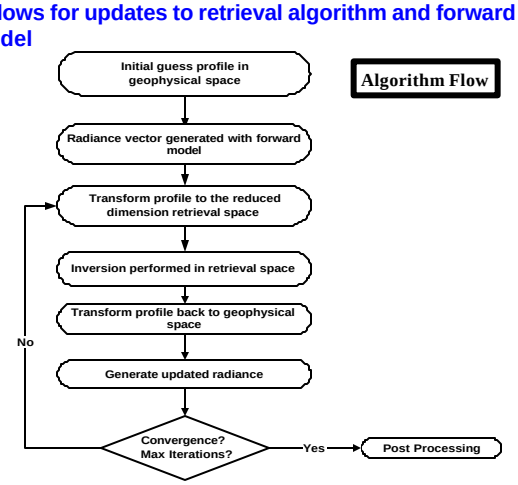
- Retrieval code has been optimized in order to comply with EDR latency requirements
- First step in optimization procedure: Benchmark and profile code
  - •Forward model and inversion procedure largest timings per iteration
- Methods implemented to decease timing:
  - • Optimize matrix and inversion routines
  - • Generate subsets of channels
    - •Used optimal selection methods
  - •Regenerate OSS optical depth tables using recently developed generalized training method
    - •Standard OSS: Localized training for each CrIS channel
    - •Generalized training: Train groups of channels simultaneously, channel correlations

NPOESS CriMSS EDR Retrieval Algorithm

- *Retrieval flow*:
  - • Retrieval temperature and water vapor profiles using ATMS data only
  - • Generate initial cloud-cleared radiance
  - • Retrieval profilesusing both CrIS and ATMS data using cloud-cleared radiance
    - •ATMS only retrieval → initial guess
    - •Iterate: until radiance convergence
      - • Generate cloud-cleared radiance
      - • Generate new EDR profile



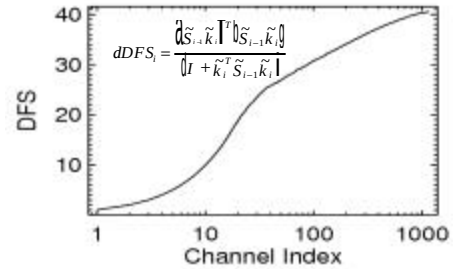
- *EDR Algorithm: Features*
  - •Non-linear iterative physical retrieval method with radiometric and geophysical constraints
  - •OSS fast radiative transfer model
  - •Simultaneous retrieval of required atmospheric and surface parameters.
  - •Empirical Orthogonal Function (EOF) decomposition of retrieval parameters
    - •Retrieval performed in reduced dimension space.
  - •Modularized software developed:
    - •Allows for updates to retrieval algorithm and forward model



Channel Selection

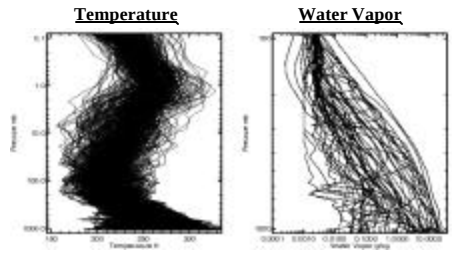
Selection Method

- Information content approach: Degrees of freedom for signal (DFS) (Rodgers 1996)
  - Sequentially sort channels by their contribution to the DFS
  - Pick desired number of channels from sorted set



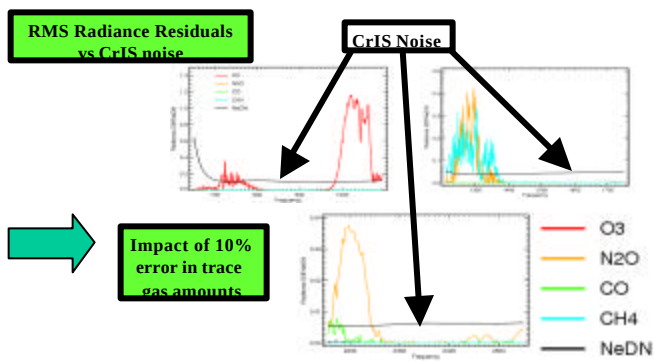
Training Profiles

- Requires variable training set:
  - Used to generate Jacobians
  - Same set used for OSS training
  - 52 ECMWF temperature and water vapor profiles
  - Randomly perturb the temperature profile to maximize variability
  - Flat emissivity: randomly varied from 0.8-1.0



Selection Pool

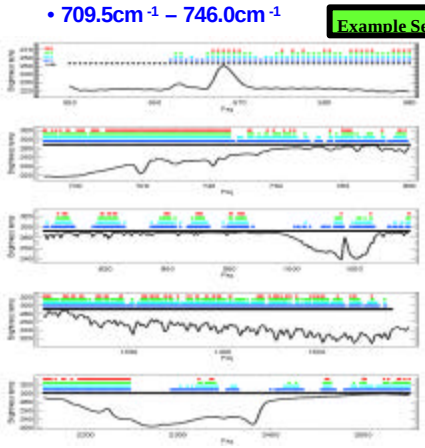
- Can pre-select/exclude channels from selection pool
  - Include channels from previous selection
  - Exclude channels:
    - Impacted by NLTE
    - Sensitive to particular molecular species
    - With spectroscopy/line shape errors



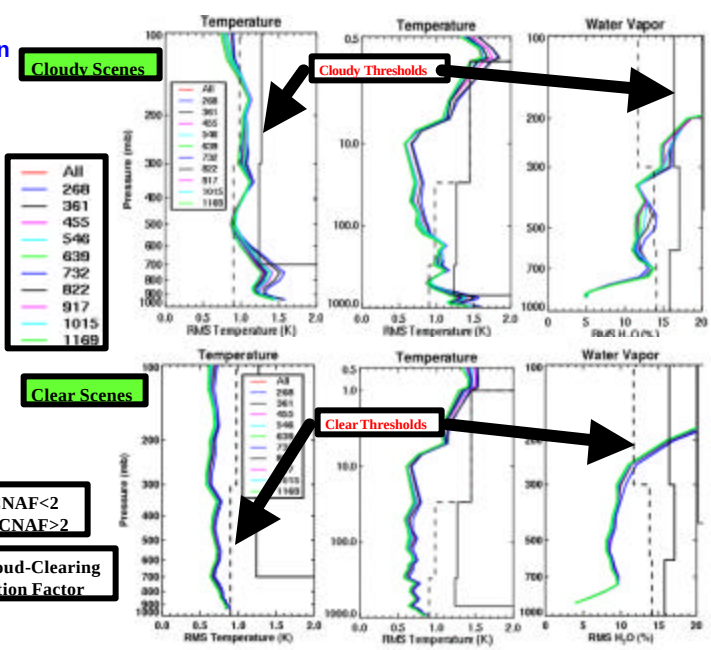
Example Selection

- Used 1169 out of the 1305 CrIS channels in the selection pool(excluded 1590cm $^{-1}$ – 1800cm $^{-1}$)
  - Initially sort channels using DFS method
  - Pick desired number up to total
  - Include cloud-clearing regions
    - 709.5cm $^{-1}$ – 746.0cm $^{-1}$

Example Selections



RMS Retrieval Errors



Clear: CCNAF<2
Cloudy:CCNAF>2

CCNAF=Cloud-Clearing Amplification Factor

Generalized Training

Optimal Spectral Sampling (OSS) Method

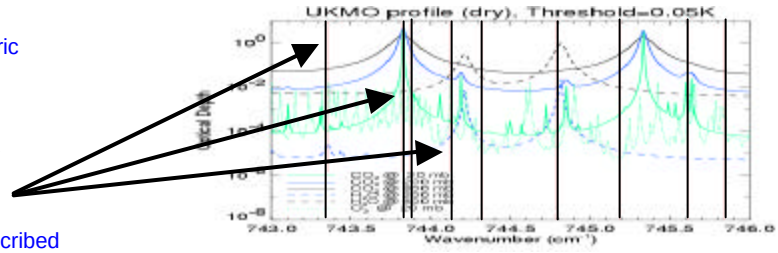
- OSS fast forward model
  - Channel radiance for inhomogeneous atmospheric path represented by weighted sum over specific frequencies or "nodes"

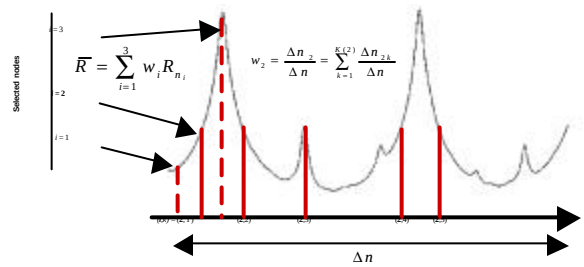
$$\overline{R} = \int_{\Delta n} f(n)R(n)dn \cong \sum_{i=1}^{N} w_i R(n_i); \qquad ?_i \in \Delta n$$

  - Automated search for smallest subset of **nodes** and weights for which the error is less than a prescribed tolerance

$$\left\{(n_i, w_i) \;\; i = 1,..,N\right\} \qquad e_N = \sum_s \left[R^s - \sum_{i=1}^{N} w_i R_{n_i}^s\right]^2$$

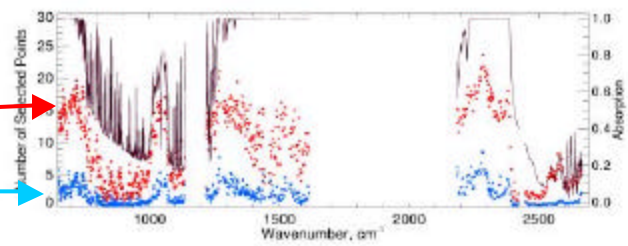
  - In the training, radiances calculated with a line-by-line model (e.g. LBLRTM, GENLN) using a globally representative ensemble of atmospheres, surface conditions, viewing angles, etc..
  - Radiance training fast
    - Planck function accounted for exactly



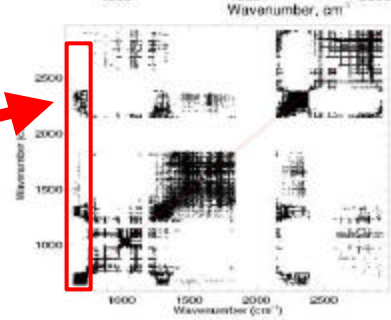


Localized versus Generalized Training

- ***Localized training*** **(benchmark) :**
  - **operates on individual channels, one at a time – node redundancy due to overlapping ILS**
- **CrIS (1305 channels):**
  - **Average # nodes per channel: ~7 nodes/channel**
  - **Total number of nodes/number of channel (i.e. no redundancy) = 3.5 nodes/channel**

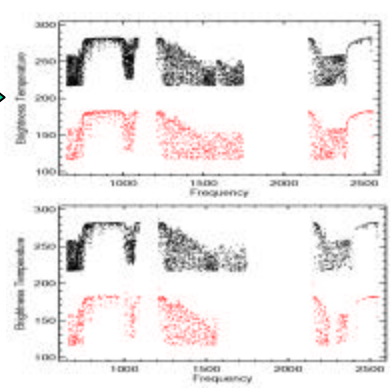


- ***Generalized Training*** **:**
  - **operates on groups of *N* channels (up to full channel set)**
  - **Exploits node-to-node correlation to minimize total number of nodes across a spectral domain**
  - **Results in significant increase in number of points in any given channel**



Radiance Correlation

- **Generated new OSS tables using the generalized training method**
  - **For full CrIS channel set**
    - **Localized training: *4599 nodes***
    - **Generalized training: *1286 nodes***
  - **Combined with channel selection: used a subset of 639 channels and performed the OSS generalized training**
    - **For the 639 subset: *3029 nodes***
    - **Localized training: *855 nodes***
    - **Generalized training:**



Localized: full set

Generalized: full set

Localized: Selected set

Generalized: Selected set

Timing Updates

- Timing optimization methods:
  - Code modifications
    - Modified the inversion methods
      - Implemented Cholesky Factorization method
      - Eliminates matrix inversion
      - *Speedup factor~1.2*
    - Switched to intrinsic F90 matrix multiplication routines
      - *Speedup factor~1.4* (with inversion update)
  - Generalized training for OSS tables
    - Reduced the total number of nodes
    - Increased the number of nodes per channel
    - Overall drop in timing but not linear
    - *Speedup factor~2.0* (with matrix/inversion updates)
  - Channel selection
    - Localized trained OSS tables
    - Timings for {300, 500, 700, 900} channels
    - Add cloud clearing channels
    - Timing factors include matrix/inversion optimization
    - *Speedup factors ~{2.5,2.0,1.8,1.6}*
  - Combine Channel selection and generalized training
    - OSS tables generated using the generalized training method
    - Timings for {300, 500, 700, 900} channels
    - Add cloud clearing channels
    - Timing factors include matrix/inversion optimization
    - *Speedup factors ~{2.8,2.6,2.3,2.1}*
    - ;

Matrix/inversion updates

Process	Baseline	Optimized Inversion Routines	Optimized Matrix Multiplication	Generalized Training OSS Table
cloud clearing	0.024	0.024	0.023	0.022
Inversion Pre-process	0.074	0.074	0.049	0.049
Inversion	0.073	0.011	0.011	0.012
MW RT	0.002	0.002	0.002	0.002
IR RT	0.131	0.137	0.131	0.065
Total	0.304	0.248	0.216	0.150
Speedup factor	1.0	1.2	1.4	2.0
Channels/nodes	1169/4341	1169/4341	1169/4341	1169/1157

Channel selection tables were generated with matrix and inversion optimized code

MW RT: OSS microwave routine
IR RT: OSS infrared routine

Process	Channel selection 300+CC	Channel selection 500+CC	Channel selection 700+CC	Channel Selection 900+CC	Channel Selection 1169+CC
cloud clearing	0.023	0.023	0.023	0.023	0.023
Inversion Pre-process	0.018	0.025	0.032	0.040	0.050
Inversion	0.005	0.007	0.008	0.010	0.012
MW RT	0.002	0.002	0.002	0.002	0.002
IR RT	0.075	0.092	0.108	0.119	0.126
Total	0.123	0.149	0.173	0.194	0.213
Speedup factor	2.5	2.0	1.8	1.6	1.4
Channels /nodes	361/2064	546/2735	732/3286	917/3785	1169/ 4341

Process	Channel selection 300+CC	Channel selection 500+CC	Channel selection 700+CC	Channel Selection 900+CC	Channel Selection 1169+CC
cloud clearing	0.023	0.023	0.023	0.023	0.022
Inversion Pre-process	0.019	0.026	0.033	0.040	0.049
Inversion	0.005	0.007	0.008	0.010	0.012
MW RT	0.002	0.002	0.002	0.002	0.002
IR RT	0.059	0.061	0.064	0.067	0.065
Total	0.108	0.119	0.130	0.142	0.150
Speedup factor	2.8	2.6	2.3	2.1	2.0
Channels /nodes	361/919	546/992	732/1063	917/1103	1169/ 1157

Ongoing Efforts

- Variational retrieval methods:
  - Average channel uses ~150 nodes
  - Mapping Jacobians from node to channel space partially offsets speed gain

$$d x_{n+1} = \left(\mathbf{K}_n^T \mathbf{S}_e^{-1} \mathbf{K}_n + \mathbf{S}_x^{-1}\right) \mathbf{K}_n^T \mathbf{S}_e^{-1} \left[\left(y_n - y^m\right) + \mathbf{K}_n d x_n\right],$$

where,

$\mathbf{y} = \mathbf{A}\,\tilde{\mathbf{y}}$ and

$\mathbf{K} = \mathbf{A}\,\tilde{\mathbf{K}}$

- Alternative:
  - Operate directly in node space
  - Avoids Jacobians transformation all together and reduce K-matrix size (inversion speed up)
  - for AIRS: 2378 channels -> 250 nodes

$$\tilde{\mathbf{y}}^m = \left(\mathbf{A}^T \mathbf{S}_e^{-1} \mathbf{A}\right)^{-1} \mathbf{A} \mathbf{S}_e^{-1} \mathbf{y}^m$$

$$\tilde{\mathbf{S}}_e^{-1} = \mathbf{A}^T \mathbf{S}_e^{-1} \mathbf{A}$$

$$\mathbf{dx}_{n+1} = \left(\tilde{\mathbf{K}}_n^T \tilde{\mathbf{S}}_e^{-1} \tilde{\mathbf{K}}_n + \mathbf{S}_x^{-1}\right) \tilde{\mathbf{K}}_n^T \tilde{\mathbf{S}}_e^{-1} \left[\left(\tilde{\mathbf{y}}_n - \tilde{\mathbf{y}}^m\right) + \tilde{\mathbf{K}}_n \mathbf{dx}_n\right]^{**}$$

**Equivalent to

$$\mathbf{dx}_{n+1} = \left(\mathbf{K}_n^T \mathbf{S}_e^{-1} \mathbf{K}_n + \mathbf{S}_x^{-1}\right) \mathbf{K}_n^T \mathbf{S}_e^{-1} \left[\left(\mathbf{A}\mathbf{H}\mathbf{y}_n - \tilde{\mathbf{y}}^m\right) + \mathbf{K}_n \mathbf{dx}_n\right]$$