Overview of the Suomi-NPP Science Team Activities
Presented by: Chris Barnet
With contributions from: Antonia Gambacorta

AIRS Science Team Meeting
Wednesday, Sep. 14, 2016 (Session 03, 10:40 am)
## The S-NPP Science Team

<table>
<thead>
<tr>
<th>PI</th>
<th>Affiliation</th>
<th>Area of study</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aumann, Hartmut</td>
<td>NASA/JPL</td>
<td>Analysis of AIRS and CrIS cloudy radiances and propagation of errors into products</td>
</tr>
<tr>
<td>Barnet, Chris</td>
<td>STC</td>
<td><strong>ST lead</strong>, Develop sequential O-E approach based on NUCAPS algorithm, called CLIMCAPS</td>
</tr>
<tr>
<td>Cady-Pereria, Karen &amp; Helen Worden</td>
<td>AER &amp; UCAR</td>
<td>Develop NH3 &amp; CO retrieval algorithms</td>
</tr>
<tr>
<td>Lambbrigtsen, Bjorn</td>
<td>NASA/JPL</td>
<td>ATMS-only level-1 and level-2 products</td>
</tr>
<tr>
<td>Moncet, Jean-Luc</td>
<td>AER</td>
<td>Develop simultaneous O-E approach based on CrIMSS-EDR algorithm for CCR, T/q/O3</td>
</tr>
<tr>
<td>Susskind, Joel</td>
<td>NASA/GSFC</td>
<td>Apply AIRS v6 algorithm to CrIS/ATMS</td>
</tr>
</tbody>
</table>
**Sounder Lead Activities**

- We hold monthly telecons, usually last Monday of the month
  - All presentations and discussion are archived
  - Contact barnet@stcnet.com to get on the invite list
- Encourage open discussion on objective evaluation methodology for climate products and sounding topics
- Coordinate with both the NASA-funded CrIS Calibration Team (Hank Revercomb, Larrabee Strow, Dave Tobin) and NOAA-funded CrIS Cal/Val Team (Yong Han’s team)
- Attend EDOS/SIPS meetings (includes all NPP disciplines)
- I am also the co-lead for NOAA JPSS *Sounding Initiatives* and an SME for operational NUCAPS algorithm
  - Allows synergy between NASA and NOAA S-NPP activities
  - Acquiring datasets of extreme events (*e.g.*, 2016 El Nino)
We provided guidance on a number of flight topics

- CrIS full spectral resolution: justification and implementation
  - Select channels (see Jonathan Smith’s talk, 3:20 pm today)
  - Evaluation of carbon monoxide retrieval (see Nadia Smith, 9:20 am Thursday)
  - Receipt and packaging of UMBC SARTA
- ATMS Scan Motor reversal guidance
  - Keep ATMS alive as long as possible (now 2 reversals/orbit)
  - Prepare for loss of ATMS (NUCAPS CrIS-only mode)
- Discussion on improvements to CrIS on future satellites
  - Spectral gap filling (allows intercal and other trace gases)
  - Smaller FOV’s (smaller 3x3 or NxN approaches)
- ATMS and CrIS co-alignment on JPSS-2 satellite
  - Decision to rotate ATMS to improve alignment across scan set
- Investigating and justifying the need for level-1a product
  - We are doing a cost-benefit analysis of archiving L1A
• Sounder SIPS has produced sample NASA level 1 for both ATMS and CrIS radiances with the latest calibration
  – Co-located in a 45 scanset NETCDF format
    • data have the “look and feel” of AIRS products
    • files were evaluated and will be ready for production in the near future
    • (next 2 talks by Steve Friedman's and Evan Manning's )
• GSFC has delivered their v6.29 algorithm that can run both AIRS/AMSU and CrIS/ATMS (see Joel Susskind's talk at 2:00 today)
• STC has delivered a CrIS/ATMS pre-processor code
  – ability to prepare data for both the GSFC and STC retrieval codes
  – creates co-located granule files for both ECMWF (spatial co-location), GFS (spatial and temporal co-location), and Merra-2 reanalysis (spatial and temporal co-location) to support algorithm comparisons
  – delivered NUCAPS retrieval output for a focus day along with GFS forecast and Merra-2 reanalysis co-located in space and time to CrIS
  – STC has recently installed NUCAPS/CLIMCAPS on the Sounder SIPS
The JPL/SIPS has done a comparison between the GSFC retrieval for both AIRS and CrIS, the NUCAPS retrieval for CrIS, ECMWF, GFS, and Merra-2. Provides a foundation for objective inter-comparisons. (Van Dang's talk at 4:00 pm)

STC is working on the CLIMCAPS algorithm (Antonia Gambacorta's talk at 2:30 pm)
  – Formally CHIMERA – had to change the name

AER is preparing an algorithm inter-comparison testbed (Alan Lipton talk at 2:20 pm) that includes the CrIMSS IDPS retrieval

AER is also providing ammonia and carbon monoxide retrievals. (part of Vivienne Payne's talk 11:40 am Thursday)

We have made progress on defining the ATMS-only retrieval module (see Bjorn Lambrigtsen, Evan Fishbein, Mathias Schreier, Antonia Gambacorta talks today at 4:40-6:00 pm)

George Aumann has been making radiometric comparisons (see talks at 1:40 pm today, 3:00 pm Thursday)
• (NASA Terra/Aqua) I have invited Bill Irion to participate in S-NPP algorithm discussions and evaluations of cloud clearing and *a-priori* choices *(see Thursday 2:20 pm talk)*
• (NOAA/NASA funding) Larrabee Strow is close to delivery of the high spectral SARTA forward model for CrIS
• (NASA) Employ/evaluate the MEASURES CAMEL product *(Eva Borbas talk, 3:00 pm today)*
• (NOAA) Characterization of NUCAPS methane and carbon monoxide trace gas products for operational applications *(Nadia Smith talk 9:20 am, Thursday)*
• (NOAA) Participated in Pacific field campaigns (Atmospheric River and El Nino Rapid Response). Over 1500 dropsondes have been acquired in extreme weather & climate events.
Let’s define a few terms

- The O-E solution can be written as:

\[
X_j^i = X_j^A + \left[ K_{j,n}^T \cdot N_{n,n}^{-1} \cdot K_{n,j} + C_{j,j}^{-1} \right]^{-1} \cdot K_{j,n}^T \cdot N_{n,n}^{-1} \cdot [R_{n}^{obs} - R_n(X_j^{i-1}) + K_n,j \cdot (X_j^{i-1} - X_j^A)]
\]

A-priori is “pivot point” and immediately replaces the 1st guess.
Solution “blends” measurements and a-priori knowledge.
Measurement (O-C) covariance
A-priori covariance defines amount of regularization.

- 1st guess can only affect Jacobian and the rate of convergence.

- A-priori is defined as Rodgers 1977.
# Summary of algorithms to characterize

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Susskind</th>
<th>AER</th>
<th>CLIMCAPS</th>
<th>Irion</th>
</tr>
</thead>
<tbody>
<tr>
<td>Regularization</td>
<td>SVD</td>
<td>O-E</td>
<td>O-E</td>
<td>O-E</td>
</tr>
<tr>
<td>Alg. type</td>
<td>sequential</td>
<td>Simultaneous/sequential</td>
<td>sequential</td>
<td>simultaneous</td>
</tr>
<tr>
<td>Clouds</td>
<td>Cloud clearing</td>
<td>Cloud clearing</td>
<td>Cloud clearing</td>
<td>Solve f/cloud</td>
</tr>
<tr>
<td>A-priori for T(p), q(p)</td>
<td>Neural Net</td>
<td>Climatology f/ multiple sources</td>
<td>Climatology &amp; MERRA-2</td>
<td>ECMWF</td>
</tr>
<tr>
<td>A-priori for emissivity</td>
<td>Borbas</td>
<td>Fit to Zhou database ?</td>
<td>MEASURES CAMEL</td>
<td>Borbas</td>
</tr>
<tr>
<td>A-priori for trace gases</td>
<td>Climatology, No covariance</td>
<td>Climatology w/ covariance</td>
<td>Climatology w/ covariance</td>
<td>Climatology w/ covariance</td>
</tr>
<tr>
<td>Error Propagation</td>
<td>Diagonal</td>
<td>T/q, Ts/ε, NH₃, CO steps</td>
<td>3-6 eigenvector</td>
<td>n/a</td>
</tr>
<tr>
<td>Error estimates</td>
<td>Parametric fit to ECMWF</td>
<td>O-E</td>
<td>Propagated O-E</td>
<td>O-E</td>
</tr>
</tbody>
</table>
## Table 1: Summary of Level.2 Algorithms to be studied as part of NPP Science Team Activities

<table>
<thead>
<tr>
<th>PI</th>
<th>Lambrigtsen</th>
<th>Susskind</th>
<th>Barnet</th>
<th>Moncet</th>
<th>Cady-Pereira</th>
<th>Irion</th>
</tr>
</thead>
<tbody>
<tr>
<td>affiliation</td>
<td>JPL</td>
<td>GSFC</td>
<td>STC</td>
<td>AER</td>
<td>AER</td>
<td>JPL</td>
</tr>
<tr>
<td>funding</td>
<td>NPP</td>
<td>NPP</td>
<td>NPP</td>
<td>NPP</td>
<td>NPP</td>
<td>NPP</td>
</tr>
<tr>
<td>ATMS</td>
<td>ATMS FOV</td>
<td>CrIS FOR</td>
<td>CrIS FOR</td>
<td>CrIS FOR</td>
<td>n/a</td>
<td>n/a</td>
</tr>
<tr>
<td>CrIS</td>
<td>n/a</td>
<td>CrIS FOR</td>
<td>CrIS FOR</td>
<td>CrIS FOR</td>
<td>CrIS FOV</td>
<td>CrIS FOV</td>
</tr>
<tr>
<td>Regularization</td>
<td>O-E</td>
<td>SVD</td>
<td>O-E</td>
<td>O-E</td>
<td>O-E</td>
<td>O-E</td>
</tr>
<tr>
<td>Alg. Type</td>
<td>Sequential</td>
<td>Sequential</td>
<td>Sequential</td>
<td>Simultaneous</td>
<td>Sequential</td>
<td>Simultaneous</td>
</tr>
<tr>
<td>Alg. Heritage</td>
<td>AIRS ST</td>
<td>AIRS ST v6+</td>
<td>AIRS ST v5.9, NUCAPS-IASI</td>
<td>CrIMSS EDR</td>
<td>TES</td>
<td>TES</td>
</tr>
<tr>
<td>Cloud Clearing</td>
<td>n/a</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>T/q a-priori</td>
<td>NCEP Climatology</td>
<td>Neural Net</td>
<td>Climatology and Merra-2</td>
<td>Climatology for O3</td>
<td>AER product</td>
<td>ECMWF</td>
</tr>
<tr>
<td>Trace gas a-priori</td>
<td>n/a</td>
<td>Climatology</td>
<td>Climatology</td>
<td>Climatology for O3</td>
<td>Climatology</td>
<td>Climatology</td>
</tr>
<tr>
<td>Error estimate</td>
<td>O-E</td>
<td>ECMWF regression</td>
<td>O-E</td>
<td>O-E</td>
<td>O-E</td>
<td>O-E</td>
</tr>
<tr>
<td>Averaging Kernels</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Execution Time (per FOR)</td>
<td>~5 ms/FOR (MIT)</td>
<td>~150 ms/FOR</td>
<td>~200 ms/FOR</td>
<td>?</td>
<td>?</td>
<td>~15 sec/FOV</td>
</tr>
</tbody>
</table>

Abbreviations: SVD=Singular Value Decomposition, O-E=Optimal Estimation, FOV=field of view, FOR=field of regard (CrIS set of 3x3 FOVs)
Simultaneous OE  |  Sequential OE
--- | ---
Solve all parameters simultaneously. | Solve each state variable (e.g., T(p)), separately.
O-C error covariance can be simpler (does not require propagation from one step to another) | O-C error covariance is computed for all relevant state variables that are held fixed in a given step. Retrieval error covariance must be propagated between steps.
Each parameter is derived from all channels used (e.g., can derive T(p) from CO2, H2O, O3, CO, … lines). | Each parameter is derived from the best channels for that parameter (e.g., derive T(p) from CO2 lines, q(p) from H2O lines, etc.). More linear.
A-priori must be rather close to solution, since state variable interactions can de-stabilize the solution. Covariance must contain cross-terms (e.g., dT/dq, dT.dO3) | A-priori can be simple for hyperspectral and, therefore, covariance can be large, more signal can be derived from the radiances
Has larger state matrices (all parameters solved) and O-C covariance matrices (all channels used). Inversion of large matrices is computationally expensive. | State matrices are small (largest is 25 T(p) parameters) and O-C covariance matrices of the channel subsets are quite small. Very fast algorithm. Encourages using more channels.
As we move from SVD to O-E we need to decide on a-priori

<table>
<thead>
<tr>
<th>Type of a-priori</th>
<th>regression</th>
<th>Static climatology</th>
<th>forecast</th>
<th>reanalysis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vertical structure</td>
<td>High, derived from radiances</td>
<td>Low, Smooth</td>
<td>High, derived from model and all obs</td>
<td>High, derived from model and all obs</td>
</tr>
<tr>
<td>Spatial &amp; temporal structure</td>
<td>high</td>
<td>Smooth</td>
<td>Very high</td>
<td>Very high</td>
</tr>
<tr>
<td>Error covariance</td>
<td>small</td>
<td>large</td>
<td>small</td>
<td>medium</td>
</tr>
<tr>
<td>Relative impact of Radiances</td>
<td>Low, IC is conflated (a tautological error – R’s used 2x)</td>
<td>Very high, all structure comes from instrument</td>
<td>Very low, fine structure from forecast, tautological error is f(t)</td>
<td>Relatively low, fine structure from reanalysis, weak tautological error</td>
</tr>
</tbody>
</table>

NOTE: When relative impact of radiances is low, you cannot remove errant structures
Choice of \textit{a-priori} is application dependent

- My goal for S-NPP ST is to intercompare sounding concepts
  - Impact of \textit{a-priori} assumptions on hyperspectral retrievals
  - Test our ability to quantify retrieval information content and error
- Discussion of \textit{a-priori} has been a topic in our community for over 40 years (see discussion at the end of Rodger's 1977 – 1pg shown on right)
- Choice of the relative weight of the \textit{a-priori} is important to characterize and communicate to our users
QUESTIONS?
Algorithm Philosophy

• Algorithm and code should be open source
• Algorithm should function on all operational modern hyperspectral and advance microwave sounder space-borne instruments
  – Minimize instrument dependent features
  – Exploit the full information content of the measurements
    • Ability to discriminate between physical correlations (e.g., climate sensitivity of dq/dT) and spectral correlations induced by measurements (e.g., dq/dT induced by spectroscopy)
• Minimize dependence of things we don't know
  – Minimize sensitivity to clouds
    • Exploit microwave information
    • IR cloud forward models are not robust (in my opinion, but some day soon this will be false)
    • Sensitivity of radiances to cloud parameters (particle sizes and shapes, vertical density) are highly non-linear
    • cloud parameters  are not well constrained by infrared or microwave sounder measurements alone
  – Minimize Sensitivity of products to interfering signals
    • $dT$, $dq$, $dT_{skin}$ co-vars with cloud signals
    • $dT$ co-vars w/ $dq$, $dO_3$, ... for IR, $dT$ co-vars with $O_2$ for MW
    • $dq$ co-vars w/ $dT$, $dCH_4$, $dSO_2$, ... for IR
      – $dq$ is significantly more linear for MW
    • If ignored, this “spectral” covariance can confound measurement of natural correlations (i.e., Earth physical correlations)
Philosophy 3/3

• Desire a global, all season, all sky, all regions, retrieval
  – avoid regional or highly tailored a-priori terms
  – avoid datasets that are not available or not skillful in remote regions

• Derive formal and traceable error estimates
  – have either averaging kernels or error covariance output for each product
  – algorithm should fully characterize inter-correlation of products induced by retrieval

• Desire a real time (weather) and re-processing (climate) capability
  – avoid algorithms that are computationally intensive (either in CPU or memory requirements) if they do not add sufficient skill
  – avoid datasets with high latency (weather)