Forward Modeling for
Microwave and Infrared Remote Sensing:
Spectroscopic Issues and Line-by-Line Modeling

Tony Clough

and a host of colleagues

Joint Center, Camp Springs, MD
15 Sep 2010
LBL Heritage and Presentation Outline

<table>
<thead>
<tr>
<th>Code</th>
<th>Organization</th>
<th>Description</th>
<th>Year</th>
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</thead>
<tbody>
<tr>
<td>FASCODE</td>
<td>AFGL</td>
<td>Fast Atmospheric Signature CODE</td>
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<tr>
<td>LBLRTM</td>
<td>AER</td>
<td>Line By Line Radiative Transfer Model</td>
<td>1983</td>
</tr>
<tr>
<td>LBL_CRA</td>
<td>CRA</td>
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<td>2010</td>
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</table>

Outline

• Emphasis on Physics
• Background and Intellectual Underpinnings
• Line Shape
• Line Coupling
• Validation Issues
• Validation Cases
  - AERI
  - IASI
  - To Do List
• Summary
## Related Models

<table>
<thead>
<tr>
<th>Model</th>
<th>Method</th>
<th>Authors</th>
</tr>
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<tbody>
<tr>
<td><strong>LBLxxx</strong></td>
<td></td>
<td>Clough et. al.</td>
</tr>
<tr>
<td><strong>CHARTS</strong></td>
<td>Multiple scattering</td>
<td>Moncet and Clough</td>
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<tr>
<td></td>
<td>Adding Doubling Method</td>
<td></td>
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<tr>
<td><strong>MonoRTM</strong></td>
<td>MonochromRTM for limited # of frequencies</td>
<td>Boukabara, Cady-Pereira and Clough</td>
</tr>
<tr>
<td></td>
<td>e.g. microwave</td>
<td></td>
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<td><strong>DISORT</strong></td>
<td>Multiple Scattering</td>
<td>Stamnes and Wiscombe</td>
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<td>Discrete Ordinate Method</td>
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<td><strong>RRTM</strong></td>
<td>Rapid RTM</td>
<td>Mlawer and Clough</td>
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<td>General Circulation Models</td>
<td></td>
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<tr>
<td><strong>OSS</strong></td>
<td>Optimal Spectral Sampling</td>
<td>Moncet</td>
</tr>
<tr>
<td><strong>MT_CKD</strong></td>
<td>Continuum</td>
<td>Mlawer, Payne and Clough</td>
</tr>
</tbody>
</table>

* adjoint easily developed due to coding attributes (next slide)

**Physics consistent with LBLxxx in these models !**
Acceptance of RRTM by the GCM community is a direct consequence of the acknowledged accuracy of LBLRTM.
LBL Model Attributes

• **Computational Accuracy**

<table>
<thead>
<tr>
<th></th>
<th>Voigt Line Shape</th>
<th>Planck Fn</th>
<th>Layer Merging</th>
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<th>Radiance</th>
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• **Computational Gain**

<table>
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<th>Line Coupling&lt;sup&gt;2nd&lt;/sup&gt;</th>
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<td>10x</td>
<td>10x</td>
<td>2x</td>
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*Computational gain can be utilized to do more complicated problems in the same amount of time*

• **Attributes**

- Linear Algebra wherever possible
- Piecewise continuous wherever possible
- Planck Fn ‘linear in tau’ across inhomogeneous layer
- Voigt Fn obtained as a linear combination of precalculated functions
- Units: cgs
- Line Coupling (second order)
- NonLTE
- Analytic Derivatives
- Logical structure of high order
- Modular and proven very flexible
- Coding: Horrendous
Formalism for LBL Calculations

- Validity from Microwave through Solar UV
- Detail Balance across entire extent of the line
  - Radiance = Planck_Fn * [ 1 - Transmittance ]

A Bit of History: With a nod to heroes of the profession!

Problem: (≈1972)
Incoherent understanding of line shape associated with binary collisions
What is the validity of the impact line shape?
What is the line shape far from line center that satisfies the physical constraints?

Development of a Water Vapor Continuum Model (Clough and Kneizys 1975)
- Phillip Anderson thesis (student of Van Vleck) (1950)
- Huber and Van Vleck I (1966)
- Huber and Van Vleck II (1972)
- John Van Vleck (Rev Mod Phys; 1978)
Formalism for LBL Calculations II

\[ k(\nu) = \nu \frac{1 - e^{-\frac{hc\nu}{kT}}}{1 + e^{-\frac{hc\nu}{kT}}} \quad \text{Im} \< \phi(\nu) + \phi(-\nu) > \]

\[ k(\nu) = \nu \tanh\left(\frac{hc\nu}{2kT}\right) \quad \text{Im} \< \phi(\nu) + \phi(-\nu) > \]

\[ \text{radiation field} \quad \text{molecular system} \quad \text{radiation interaction} \]

\[ \text{line shape} \]

\[ <\text{symmetrized spectral density function}> \]

- Radiation balance is satisfied over the full extent of the spectral line irrespective of accuracy of \( \phi(\nu) \)!
- F-sum rule rigorously satisfied: integral over \( \nu \) value of the band strength
- Led to the development of the CKD continuum model

Impact Result:

\[ \approx \nu \left\{ 1 - e^{-\frac{hc\nu}{kT}} \right\} \frac{1}{\pi} \left[ \frac{\alpha_i P}{(\nu_i + \nu)^2 + (\alpha_i P)^2} + \frac{\alpha_i P}{(\nu_i - \nu)^2 + (\alpha_i P)^2} \right] \]

Microwave:

\[ \approx \frac{hc^2}{2kT} \quad <g_i^\prime(T) > \frac{1}{\pi} \left[ \frac{\alpha_i P}{(\nu_i + \nu)^2 + (\alpha_i P)^2} + \frac{\alpha_i P}{(\nu_i - \nu)^2 + (\alpha_i P)^2} \right] \]

Van Vleck - Weisskopf

Gross, etc. \ xxx

Infrared:

\[ \approx \nu \quad <g_i^\prime(T) > \frac{1}{\pi} \left[ \frac{\alpha_i P}{(\nu_i - \nu)^2 + (\alpha_i P)^2} \right] \]

Lorentz
**LBL Model**

```
Atmosphere (lblatm)

Loop over Layers (xlayer)

Opt_Dpth (hirac)

Radiance (xmerge)

Postprocessing (e.g. fftscan)
```

**Databases**

Prestored Atmospheres

- Line parameters
- Partition Function
- Continuum
- NonLTE State Populations
- Cross Sections
- Aerosols and Clouds (absorbers)

**HiRAC**

\[ \phi(v) + \phi(-v) \]

**High Resolution Absorption Coefficient**
Impact Approximation »» Duration of Collision »» $\chi(v_i - v)$ factor

$$k(v) \approx v \left\{ \frac{1 - e^{-\frac{hc v}{kT}}}{1 + e^{-\frac{hc v}{kT}}} \right\} < S_i^\alpha(T) \frac{1}{\pi} \left[ \frac{\alpha_i P}{(v_i + v)^2 + (\alpha_i P)^2} \chi(v_i + v) + \frac{\alpha_i P}{(v_i - v)^2 + (\alpha_i P)^2} \chi(v_i - v) \right] >$$

- $S_i^\alpha(T)$
- $v_i \Rightarrow v_i + \delta_i(P, T)$
- $\alpha_i \Rightarrow \alpha_i \gamma_i^{T/T_0}$
- $\chi(v_i - v)$
- $\chi$ F$n$
Line Coupling

The task is to evaluate the collision operator in Liouville (line) space: $$[\nu - \nu_0 - i \mathbf{P} \cdot \mathbf{W}]^1$$

$$k(\nu) = \nu \tanh(\beta \nu / 2) \Im[\phi(\nu)+\phi(-\nu)]$$

$$\phi(\nu) = \frac{1}{\Pi} \sum_{jk} \mu_j < j \left| \frac{1}{(\nu - \nu_0) - i \mathbf{P} \cdot \mathbf{W}} \right| k > \mu_k \rho_k$$

diagonalize: $$(\nu_0 + i \mathbf{P} \cdot \mathbf{W})$$

$$X^{-1} (\nu_0 + i \mathbf{P} \cdot \mathbf{W}) X = \lambda' + i \lambda''$$

$$\nu - \nu_0 - i \mathbf{P} \cdot \mathbf{W} = X \left( \nu - \lambda' - i \lambda'' \right) X^{-1}$$

$$(\nu - \nu_0 - i \mathbf{P} \cdot \mathbf{W})^{-1} = X^{-1} (\nu - \lambda' - i \lambda'')^{-1} X$$

$$\phi(\nu) = \frac{1}{\Pi} \sum_{jk} \mu_j X_{jl} (\nu - \lambda'_l - i \lambda''_l)^{-1} X^{-1}_{lk} \mu_k \rho_k$$

$$= \frac{1}{\Pi} \sum_{l} \frac{(\nu - \lambda'_l) + i \lambda''_l}{(\nu - \lambda'_l)^2 + (\lambda''_l)^2} \sum_{jk} X^{-1}_{lh} \mu_k \rho_k \mu_{hl}$$

$$\Im \{ \phi(\nu) \} = \frac{1}{\Pi} \sum_{l} \frac{\lambda''_l S + S'(\nu - \lambda'_l)}{(\nu - \lambda'_l)^2 + (\lambda''_l)^2}$$

$$S', S'', \lambda', \lambda''$$

$$\mathbf{S} = \rho \mu_l^2$$

$$S' = S_l \left( 1 + g_l \left( \frac{P}{P_0} \right) \right)$$

$$S'' = S_l \, y_l \left( \frac{P}{P_0} \right)$$

$$\lambda'' = \alpha_l \left( \frac{P}{P_0} \right)$$

$$\lambda' = \nu_l + \delta_l \left( \frac{P}{P_0} \right)$$
Line Shape

Line Shape including widths, shifts and line coupling coefficients is the dominant source of error in current radiance calculations

- **Doppler**
  - Gaussian
- **Collisional**
  - Lorentzian
  - frequency of collision: \((P/T)\)
- **Voigt**
  - Convolution of Gaussian with Lorentzian
- **Duration of collision**
  - Impact approximation is just that: line wings must decay exponentially
- **Speed Dependent Voigt**
  - Doppler and Collisional processes are not independent
- **Line Coupling**
  - Collisional relaxation matrix between lines required
Thoughts on Forward Model Validation and Spectroscopy

- The atmospheric conditions for which spectroscopic parameters are required are difficult to obtain in the laboratory— for water vapor, essentially impossible (long paths-cold temperatures)
- Spectroscopy error, though small, is the dominant error in most retrievals
- Spectroscopists have been making significant progress
- The OCO experiment has been a great motivator
- A strong commitment to study line shapes was articulated at the HITRAN meeting June 2010
- Nevertheless, improved spectroscopy is needed now!

**In situ measurements are simply not adequate**

- Spatial and temporal sampling issues
- Accuracy of the measurements themselves is not adequate
- *In situ* measurements are useful: e.g. vertical structure

**My perspective is that the atmosphere will have to function as our laboratory**

- Focus on a small number of cases (10) spanning a range of atmospheric conditions
- Initial cases: night time over ocean quiet atmosphere
  
  Progressing to day time cases, land cases always with as quiet an atmosphere as possible
- Spectral residuals to follow are based on *ad hoc* changes in line parameters
  
  Progressing to retrieval of line parameters from atmospheric spectra (tuning?)
What is Truth?

- **Spectral Residuals are Key!**

- **Consistency within a band system**
  - $\nu_2$ band to investigate consistency for H$_2$O

- **Consistency between bands**
  - $\nu_2$ and $\nu_3$ bands to investigate consistency for CO$_2$

- **Consistency between species**
  - TES: temperature from O$_3$ and H$_2$O consistent with CO$_2$; N$_2$O

- **Consistency between instruments**
  - IASI
  - AIRS
  - ACE
  - TES
  - MIPAS
  - SHIS
  - NAST-I
  - AERI
Collaborators for IASI Case

- **Collaborators:**
  - M. Shephard, V. Payne, K. Cady-Pereira and J. Delamere  
    AER, Inc.
  - W. Smith and S. Kireev  
    Hampton U.
  - Extension of

  **Performance of the line-by-line radiative transfer model (LBLRTM) for temperature and species retrievals: IASI case studies from JAIVEx:**  

- **IASI Cases from JAIVEx**
  - **2007_04_19**
    » Over SGP site (surface emissivity retrieved)
    » Atmosphere
      • Clear and Homogeneous (h2o)
      • ‘Well Characterized’
  - **2007_04_20**
    » Over Gulf of Mexico 
    » Atmosphere
      • Broken Clouds and Highly Inhomogeneous (h2o)
      • Not So Well Characterized
Topics / Issues

- **Temperature**
  - **Carbon Dioxide**
    » Line Parameters: CDDDB (2008), Tashkun et al. JQSRT, 2009
    » Line Coupling: Niro et al., JQSRT, 2005 J.M.Hartmann
    ✓ Agreement between CO$_2$ $v_2$ and CO$_2$ $v_3$
    ✓ Q-Branch 667 cm$^{-1}$
    ✓ Band Head 2385 cm$^{-1}$
  - **Nitrous Oxide**
    ? Agreement between CO$_2$ $v_2$ and N$_2$O $v_3$
    » N$_2$O profile scaling required:
      19 April case: 1.04
      20 April case: 1.02

- **Methane**
  ✓ Line Coupling: Tran et al., JQSRT, 2006 J.M.Hartmann

Water Vapor

- Deserves a slide of its own
- Significant improvements but …
Introduction

IASI

- Scan Rate: 8 secs
- Scan Type: Step and dwell
- Pixel IFOV: 0.8225°
- IFOV size at Nadir: 12 km
- Sampling at Nadir: 18 km
- Earth View Pixels / Scan: 2 rows of 60 pixels each
- Swath: ± 48.98°
- Swath: ± 1066 km
- Spectral Range: 645 to 2760 cm⁻¹
- Resolution (hw/hh): 0.25 cm⁻¹
- Lifetime: 5 years
- Power: 210 W
- Size: 1.2 m x 1.1 m x 1.3 m
- Mass: 236 kg
- Data rate: 1.5 Mbps
- Radiometric Calibration: < 0.1 K

The IASI programme is led by:
Centre National d'Études Spatiales (CNES) in association with EUMETSAT.
Alcatel Alenia Space is the instrument Prime Contractor.
Strategy: to analyze the spectroscopy in the context of these red residuals
IASI 19 Apr 2007  CO$_2$ Q-Branch
Sensitivity to Upper Stratosphere

[Graph showing brightness temperature (K) vs. wavenumber (cm$^{-1}$). The graph includes multiple lines representing different models and calculations, such as tashkun Q_cpl *1.2 strat_mod and IASI.]
Voigt Parameter and Q Branch Monochromatic Spectrum

\[ \zeta = \frac{\alpha_c}{\alpha_c + \alpha_D} \]
Effect of Line Coupling on CO$_2$ Continuum

![Graph showing the effect of line coupling on CO$_2$ continuum.](image)
$\nu_3$ Bands of $\text{N}_2\text{O}$ and $\text{CO}_2$

2150 - 2500 cm$^{-1}$

LBL_CRA: $\text{N}_2\text{O}$ increased by 1.04
**CO₂ Line Coupling**

- **Line Parameters:**
  - P, Q, & R line coupling for bands of importance
  - **Niro, F., K. Jucks, J.-M. Hartmann,** Spectra calculations in central and wing regions of CO₂ IR bands. IV: Software and database for the computation of atmospheric spectra: J Quant Spectrosc Radiat Transfer., 95, 469-481.
  - Niro et al. code modified to generate first order line coupling coefficients, \( Y_i \).
  - Works in regular line by line mode with LBLRTM
  - Temperatures: 4

- **Line Shape:**
  - Impact Approximation
  - Duration of collision effects under study

- **Continuum:**
  - Band head: 2385 cm⁻¹

![Chi Function](attachment:chi_function.png)

Chi Factor

Line Coupling - Duration of Collision

Clough/Burch/Benedict based on \( \nu_3 \) band

Impact - This Work

Clough et al, 1978

Cousin (a) N₂ 296K

Cousin (c) N₂ 238K

Cousin (a) O₂ 296

Cousin (c) O₂ 238

Line Coupling

Chi Function

Wavenumber from Line Center (cm⁻¹)
Line Coupling in Methane

Tran et al., JQSRT, 2006

Ave: 0.035 K
Std: 0.250 K
Ave: -0.019 K
Std: 0.145 K
Water Vapor: ‘The Most Important Greenhouse Gas’
Critical for NWP and Climate

- **Line Strengths**
  - Laurent Coudert
    » Strong Lines: Intensities increased by ~ 5 %

- **Line Widths and Shifts / Temperature Dependence**
  - Bob Gamache & this paper

- **Line Coupling**
  - Linda Brown (accidental two line resonances)
    - Revised relaxation rates
    - First Order

- **Continuum**
  - Inextricably linked to the width
  - mt_ckd_2.4 >> 2.5 (water only)
  - Scaled in selected regions of the water band by ~5%
AERI Downwelling Radiances I

ARM NSA Site

PWV: 1.866 mm
AERI Downwelling Radiances II
ARM NSA Site

Line Coupling
AERI Downwelling Radiances III
ARM NSA Site

PWV: 1.866 mm
Water Vapor $\nu_2$ Region: Impact of Coudert Intensities
Water Vapor P-Branch: 1310 - 1410 cm\(^{-1}\)

Widths modified

Ave: 0.173 K
Std: 0.225 K
Ave: 0.044 K
Std: 0.183 K
Water Vapor P-Branch: 1400 -1500 cm\(^{-1}\)

Widths and Continuum modified

Ave: 0.372 K
Std: 0.242 K
Ave: 0.008 K
Std: 0.190 K
Water Vapor Band Center: 1530 - 1630 cm⁻¹

Line Coupling
1540 cm⁻¹

Widths and Continuum modified

Ave: -0.047 K
Std: 0.267 K
Ave: 0.007 K
Std: 0.219 K
Water Vapor R-Branch: 1640 -1750 cm⁻¹

- Widths modified
  - Ave: 0.060 K
  - Std: 0.321 K
  - Ave: 0.056 K
  - Std: 0.329 K

Line Coupling
1653 cm⁻¹
Overall Comparison of LBL_CRA with IASI

19 Apr 2007  SGP case
Summary - 1

- **Temperature**
  - **Carbon Dioxide**
    - Line Parameters: Tashkun et al. JQSRT, 2009
    - Line Coupling:
      - Niro et al., JQSRT, 2005 J.M.Hartmann
      - Q-Branch 667 cm⁻¹: Niro * 1.2
    - Band Head 2385 cm⁻¹: Robust for 19 April and 20 April (low water cases)
      - Line Coupling > Continuum
    - Good agreement between $\text{CO}_2 \nu_2$ and $\text{CO}_2 \nu_3$
  - **Nitrous Oxide**
    - Agreement between $\text{CO}_2 \nu_2$ and $\text{N}_2\text{O} \nu_3 / \text{CO}_2 \nu_3$
    - $\text{N}_2\text{O}$ profile scaling required: 19 April case: 1.04
      - 20 April case: 1.02
    - $\text{N}_2\text{O}$ shows more variability than expected
  - **Methane**
    - Residuals significantly reduced with line coupling: Tran * 1.5
      - Tran et al., JQSRT, 2006 J.M.Hartmann
Summary - 2

- **Water Vapor**
  - Sondes provide an excellent first guess / structure (nothing more)
  - **Coudert strengths**
    - Residuals unchanged; retrieved water in upper trop reduced 10%
  - Widths are the current major issue
    - Gamache widths: 350 - 1600 cm⁻¹
    - Widths of a series of weak high J low Ka P-Branch lines reduced by ~50%
  - Widths and continuum are inextricably linked
  - Three coupled lines observed so far (accidental line resonances)
  - P-Branch has much lower residuals than R-Branch. Why ???
    - Gamache Widths ???
  - 19 April 2007 case is superb for FM improvement
  - Due to the resolution of IASI there is a limit to the spectroscopic improvements that can be achieved
Summary - 3

• Next Steps
  – Resolve R-Branch Issues for water vapor
  – More Cases
    – Night time with high water
    – Day time cases for impact of NLTE on 720 cm-1 Q-Branch
  – Line Shape issues are the dominant problem
  – Spectroscopy needs greater support to take full advantage of the data
  – Thinking of the real world as our laboratory
  – Implement line parameter retrieval scheme using spectral residuals

Performance of LBL_xxx is generally gratifying
(said in not quite all modesty?)
10 years ago I wouldn’t have envisioned that we would be modeling at this level
**Line Coupling: Accidental Line Resonances**

### 400 cm⁻¹  
**Tony Clough**  

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<th>340K</th>
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### 1540 cm⁻¹  
**Linda Brown**

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### 1630 cm⁻¹  
**Linda Brown**  

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