## Forward modelling for advanced infrared sounders

Roger Saunders (Met Office, U.K.)

- What is a forward model?
- Techniques used for fast RT models
- Validation and comparison of RT models
- Examples of use of RT models
- Issues for discussion



## **Acknowledgements**

Andrew Collard, James Cameron, Jon Taylor (Met Office, U.K.)

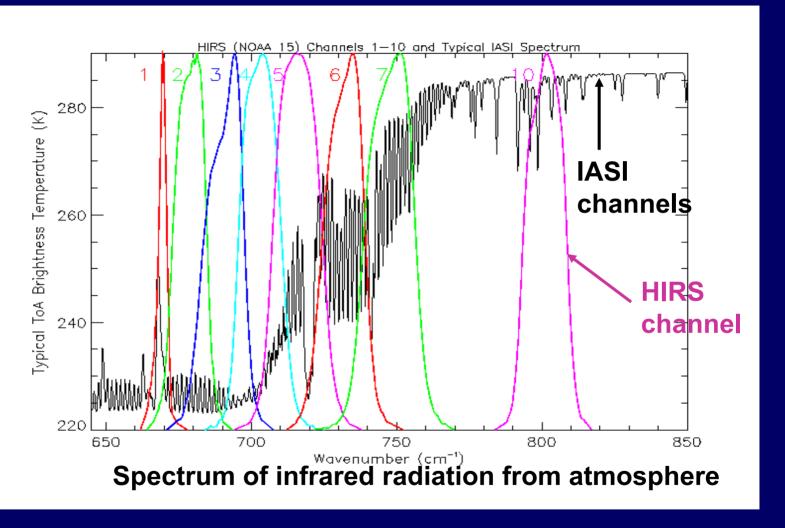
Marco Matricardi and Erik Andersson (ECMWF)

Vanessa Sherlock (NIWA)

Xu Liu (NASA) + AIRS RT modellers



## From HIRS to IASI fast models



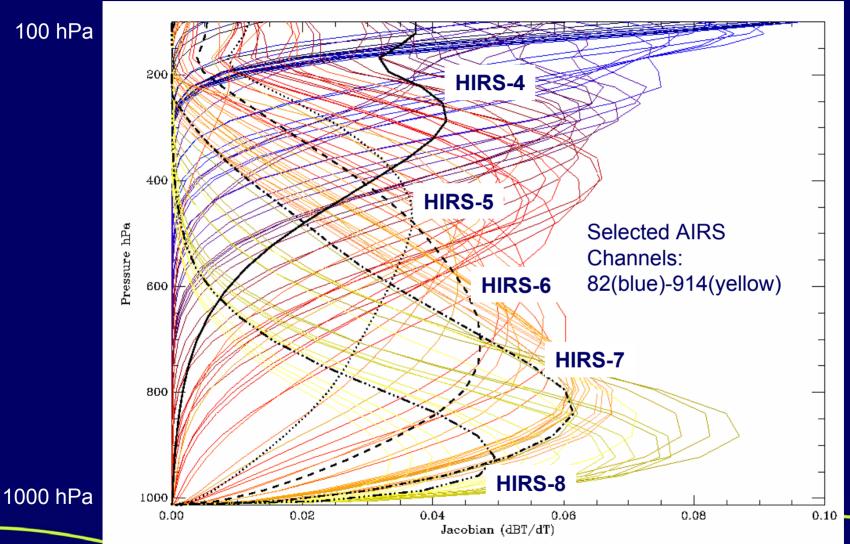
HIRS 19 channels vs IASI 8461 channels



## AIRS vs HIRS Jacobians

in the 15µm CO<sub>2</sub> band

100 hPa





### What fast RT models are used for

- Simulation of AIRS/IASI data for:
  - information content studies
  - OSSE generation
  - pre-launch ground segment tests
- Radiance assimilation in 3/4DVar
- Physical retrievals (e.g. 1DVar)
- Real time instrument monitoring
- Model validation



## IR Advanced sounders for NWP

Name	AIRS	IASI	CrIS
Instrument	Grating	FTS	FTS
Spectral range	649 –1135	Contiguous	650 –1095
(cm <sup>-1</sup> )	1217–1613	645-2760	1210 –1750
	2169 –2674		2155 –2550
Unapodized spectral resolution (cm <sup>-1</sup> )	0.5-2.25	0.35-0.5	0.625 1.25 2.5
Field of view (km)	13 x 7	12	14
Sampling density per 50 km square	9	4	9
Platform	Aqua	METOP	NPOESS
Launch date	May 2002	2005	2006 (NPP)



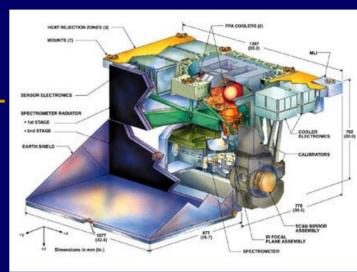
## For RT modelling must know instrument spectral response functions (ISRF)

#### **Spectrometers**

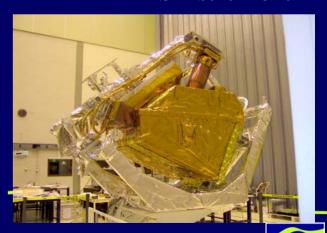
- Knowledge of actual filter responses (lab +inorbit)
- Varies with instrument temperature
- Variable for different satellites
- Correlations seen between blocks of channels

#### **Interferometers**

- Must track optical path difference as determines ISRF.
- Knowledge of self apodisation must be known (i.e. ISRF equivalent for interferometer)
- Apply known apodising function during preprocessing to facilitate forward modelling
- Known correlations across all channels from apodisation

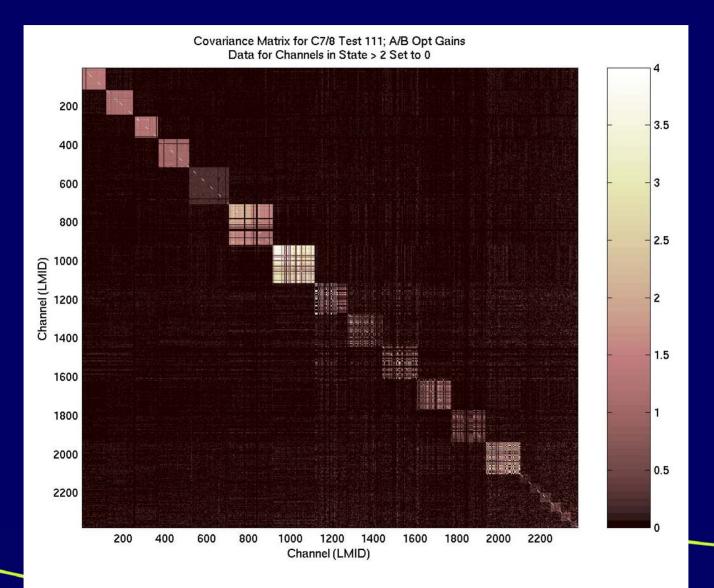


#### **AIRS** instrument



**IASI** instrument

### **AIRS channel correlations**





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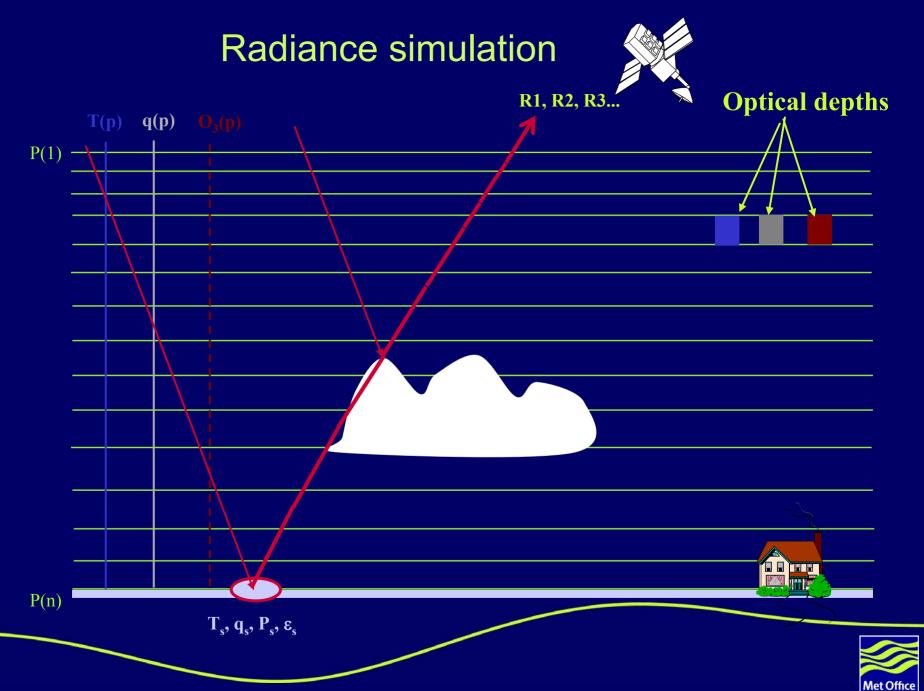


## Radiative Transfer Equation

$$\begin{split} R_{\nu} &\cong \varepsilon_{\nu} B_{\nu}(\Theta_{s}) T_{s,\nu} + \int_{p_{s}}^{0} B_{\nu}(\Theta(p)) \frac{\partial T_{\nu}(p,\theta_{u})}{\partial p} dp \\ &+ (1 - \varepsilon_{\nu}) T_{s,\nu} \int_{0}^{p_{s}} B_{\nu}(\Theta(p)) \frac{\partial T_{\nu}^{*}(p,\theta_{d})}{\partial p} dp + \rho_{\nu} T_{s,\nu} T_{\nu}(p_{s},\theta_{sun}) F_{0,\nu} \cos \theta_{sun} \end{split}$$

- The first term is the surface emission
- The second term is the upwelling thermal emssion
- The third term is the reflected downwelling radiation
- The last term is the reflected solar radiation





## Fast RT model: Terminology

$$y = H(X)$$

Where:

y is vector of radiance channels AIRS is 2378, IASI is 8461

X is state or profile vector:

$$T(p)$$
,  $q(p)$ ,  $oz(p)$ , etc on 50-100 levels  $T_s, q_s, P_s$ , + cloud

*H* is observation operator for radiance measurements and comprises:

Interpolation of model fields to observations
Fast radiative transfer model



#### What is a fast RT model?

- Used to simulate top-of-atmosphere radiances as would be measured by infrared radiometers within a few msecs
- Also provides layer to space transmittances
- Other ancillary information (e.g. overcast radiances)
- Provides Jacobians (analytic or finite difference)
- Not part of NWP model radiation scheme which provides SW/LW fluxes & heating and cooling rates



### What should an RT model include?

#### Mandatory Optional

- Clear sky transmittance and radiances
  - Variable water vapour, O<sub>3</sub>, CO<sub>2</sub>, N<sub>2</sub>O, CH<sub>4</sub>, ...
  - Include downwelling reflection
  - Include solar reflection (for SW IR channels)
- Surface emissivity model over sea and land.
- Cloudy/Aerosol radiance simulation
  - Allow different overlap assumptions and optical properties
  - Include multiple scattering from aerosols
- Be able to simulate filter radiometers and advanced IR sounders (spectrometers and interferometers)
- Compute fast and 'smooth' Jacobians
- Be also able to cope with microwave sensors so a unified model can be used in NWP systems



## Quantisation of RT model

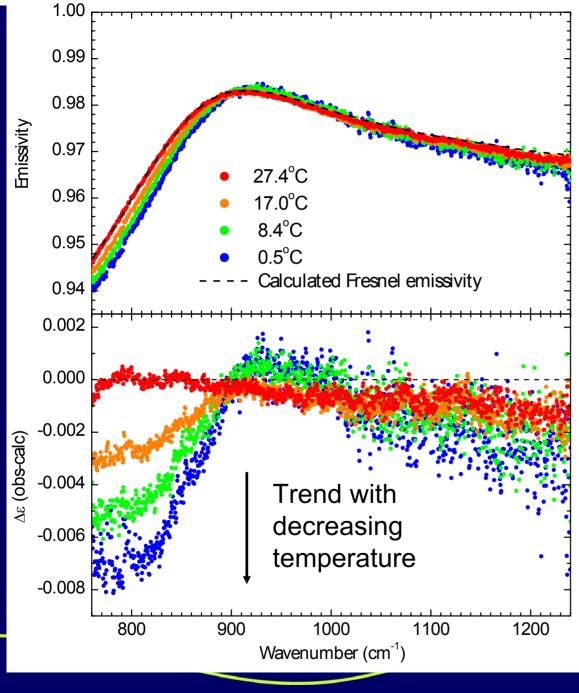
- Spectral sampling (frequency interval?)
- Number of training profiles (~50 regression, thousands for neural net)
- Profile layering (how many?) 50-100
- Computation of mean layer values (Arithmetic Mean, Curtis-Godson, etc)



### Other model components

- Surface emissivity models
  - Sea surface (e.g. Masuda/Watts) new results from a/c data
  - Land surface (e.g. Snyder) MODIS now providing new data
- Treatment of clouds
  - Infra-red
    - » Extinction coeffs and single scattering albedos as fn of freq
    - » Water and ice cloud treated separately
    - » Several overlap assumptions
- Aerosols
- Solar reflection term

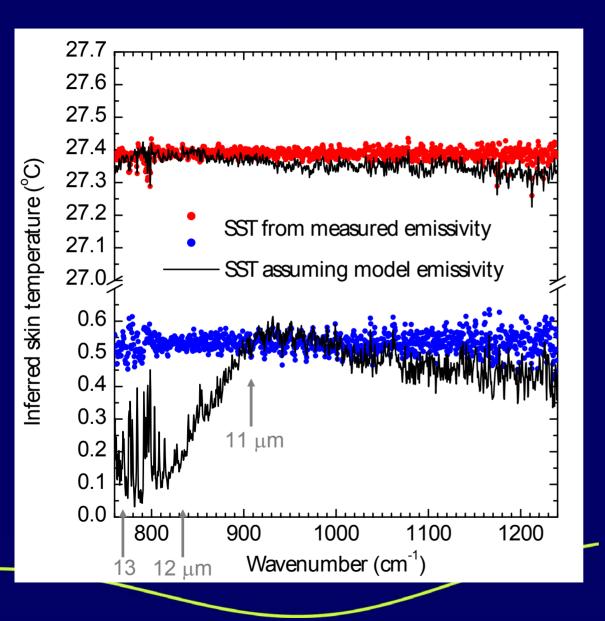




# Emissivity temperature dependence

- Pure water (zero salinity)
- No need to consider distribution of wave slopes, i.e. use Fresnel equations
- Calculated emissivity from Downing and Williams refractive indices (1975 paper, measured at 27°C)

### SST retrievals: effect of temperature



- At 27°C "SST" is retrieved consistently to within 0.1°C
- At 0.5°C the SST is underestimated by as much as 0.4°C assuming the model emissivity
- This is valid for a planar pure water surface



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### Clear sky datasets for RT models

- Some fast RT models have to be generated from a dataset of 'accurate' transmittance profiles (~50) from a diverse profile dataset
- Need to consider:
  - generation of diverse profile dataset
  - how 'accurate' transmittance profiles are generated (from Line-by-line models)
  - how fast RT model is then developed from these data



## Line by line Model parameters

- Line database (e.g. GEISA, HITRAN)
  - line freq, strength, width ......
- Line-by-line models
  - (e.g. GENLN2, LBLRTM, kCARTA, 4A ....)
- Continuum formulations (e.g. MT\_CKD, CKD2.X)
- Line mixing and non-lte effects
- Well mixed gases to include
  - (CO<sub>2</sub>), CH<sub>4</sub>, N<sub>2</sub>O, CO, CFCs, N<sub>2</sub>, O<sub>2</sub>...
- Variable gases to include
  - H<sub>2</sub>O, O<sub>3</sub>, (CO<sub>2</sub> and potentially more of above)



## Fast Model Approaches

- Linear regression (profile ⇒ optical depth)
  - On fixed pressure levels (RTTOV, PLOD, SARTA) –later slide
  - On fixed absorber overburden layers (OPTRAN)
- Physical method
  - Spectrally averaged parameters for channel (MSCFAST)
- Correlated K distribution
  - Reorder monochromatic transmittances and only retain key frequencies (Synsatrad)
- Optimal Spectral Sampling
  - Linear combination of monochromatic radiances at predefined frequencies. Uses a LUT for speed (OSS)



## Fast Model Approaches

- Neural nets
  - Uses large training set to handle non-linear relationship between T, q and radiances (LMD)
- PCA approach for advanced IR sounders
  - Redundant information in high resolution spectra and PCA is an efficient way to compress info content (see later slide) (NASA)



Predictor	Fixed gases	Water vapour	Ozone	F
$X_{j,l}$	$sec(\theta)$	$sec^2(\theta)W_r^2(j)$	$sec(\theta)O_r(j)$	S
$X_{j,2}$	$sec^2(\theta)$	$(sec(\theta)W_w(j))^2$	$\sqrt{sec(\theta)O_r(j)}$	a
$X_{j,3}$	$sec(\theta)T_r(j)$	$(sec(\theta)W_w(j))^4$	$sec(\theta) O_r(j) \delta T(j)$	n
$X_{j,4}$	$sec(\theta)T_r^2(j)$	$sec(\theta)W_r(j)\delta T(j)$	$(sec(\theta)O_r(j))^2$	
$X_{j,5}$	$T_r(j)$	$\sqrt{sec(\theta)W_r(j)}$	$\sqrt{sec(\theta)O_r(j)} \delta T(j)$	
$X_{j,6}$	$T_r^2(j)$	$^{4}\sqrt{sec(\theta)W_{r}(j)}$	$sec(\theta) O_r(j)^2 O_w(j)$	
$X_{j,7}$	$sec(\theta)T_w(j)$	$sec(\theta)W_r(j)$	$\frac{O_r(j)}{O_w(j)}\sqrt{sec(\theta)O_r(j)}$	
$X_{j,8}$	$sec(\theta) \frac{T_w(j)}{T_r(j)}$	$(sec(\theta)W_r(j))^3$	$sec(\theta) O_r(j) O_w(j)$	R
$X_{j,9}$	$\sqrt{sec(\theta)}$	$(sec(\theta)W_r(j))^4$	$O_r(j) sec(\theta) \sqrt{(O_w(j) sec(\theta))}$	
$X_{j,10}$	$\sqrt{sec(\theta)}$ $\sqrt[4]{T_w(j)}$	$sec(\theta)W_r(j)\delta T(j) \delta$	$ST(j)$ $sec(\theta) O_w(j)$	O
$X_{j,11}$	0	$(\sqrt{sec(\theta)W_r(j)})\delta I$	$T(j) \qquad (sec(\theta) O_w(j))^2$	p
$X_{j,12}$	0	$\frac{(sec(\theta)W_r(j))^2}{W_w}$	0	
$X_{j,13}$	0	$\frac{\sqrt{(\sec(\theta)W_r(j)}W_r}{W_w(j)}$	$\underline{d}_{i,j} = d_{i,j}$	, <i>j</i> −1
$X_{j,14}$	0	$sec(\theta) \frac{W_r^2(j)}{T_r(j)}$	0	
$X_{j,15}$	0	$sec(\theta) \frac{W_r^2(j)}{T_r^4(j)}$	0	

For RTTOV-8 separate out water vapour line and continuum + more trace gases

## RTTOV-7 Optical depth oredictors



## Combining transmittances

#### For monochromatic calculations:

$$au_{total} = au_{mix} imes au_{wv} imes au_{oz}$$

is valid but for sensors with broad filters it is better to compute the total transmittance as follows:

$$\tau_{total} = \tau_{mix} + \frac{\tau_{mix+wv}}{\tau_{mix}} + \frac{\tau_{mix+wv}}{\tau_{mix}}$$

The 3 terms on the RHS must be computed from an atmospheric profile of T, wv and ozone. This can be extended for other variable gases. Alternate approach now being considered:

$$\tau_{total} = \tau_{mix} \times \tau_{wvline} \times \tau_{wvcont} \times \tau_{oz} \times \tau_{xx} ... \times \tau_{corr}$$



#### **Overview of PCA for fast RTM**

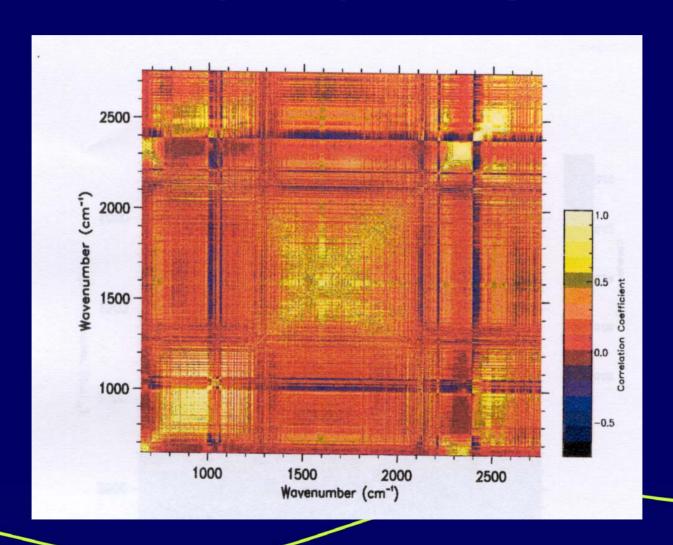
Calculates channel radiances (or transmittances) by linear combination of a set of pre-stored EOFs:

$$\vec{R}^{ch} = \sum_{i=1}^{N_{EOF}} c_i \vec{U}_i + \vec{\varepsilon} = \sum_{i=1}^{N_{EOF}} \left( \sum_{j=1}^{N_{mono}} a_j R_j^{mono} \right) \vec{U}_i + \vec{\varepsilon}$$

- EOFs  $\overline{U_i}$  are obtained by performing a Principal Component Analysis (PCA) of channel radiances under a wide range of atmospheric and observation conditions
- Coefficients  $C_i$  are predicted from a few monochromatic radiances which depend on (T, Ts, H<sub>2</sub>O and trace gases....)
- C<sub>i</sub> can be treated as super channels which contain all the essential information on a spectrum
- Provides Jacobians for both C and R
- Computational saving is more than a factor of 30 relative to channel by channel approach

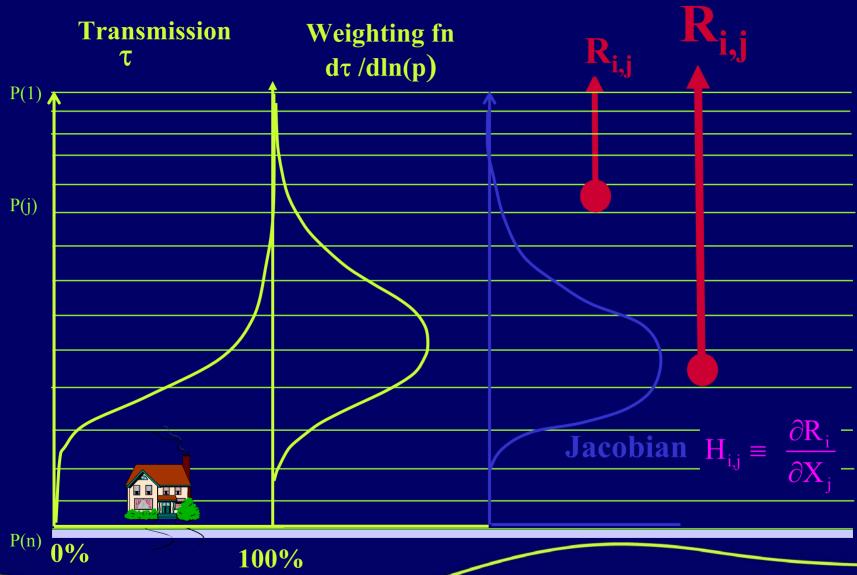


## Forward model error correlation matrix for RTIASI





### Jacobian matrix





## Jacobian/Tangent Linear/Adjoint

Operators to compute gradient of model y=H(X) about initial state X. The full Jacobian matrix H is

$$\mathbf{H} \equiv \frac{\partial \mathbf{y}}{\partial \mathbf{X}}$$

- y has dimension of number of channels and X the number of state vector variables
- H can be a large matrix if more than 1 profile at a time is operated on (hence the TL/AD operators) but for 1 profile it is *chans x levels x ngases* so is used in 1DVar applications.



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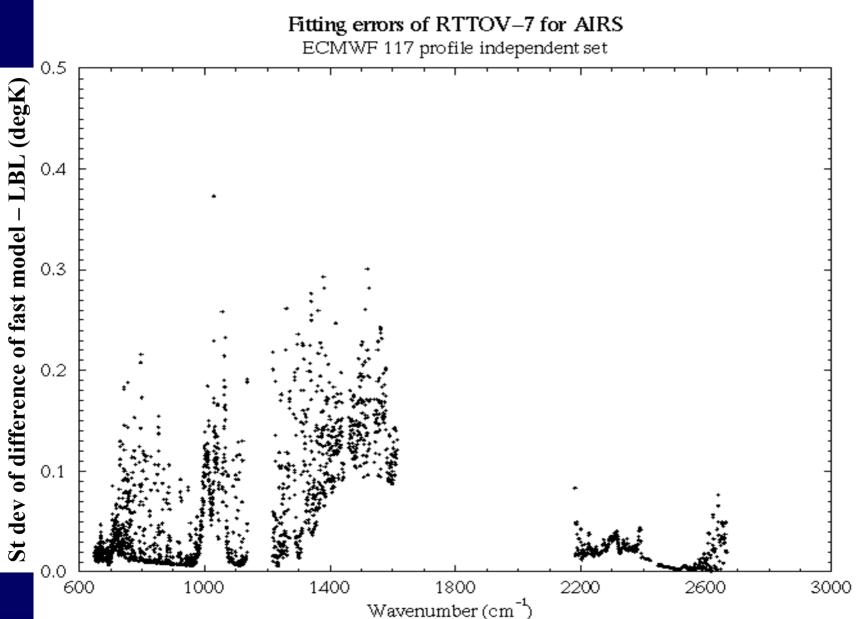


#### How to validate RT models?

- Use an independent set of profiles (e.g. ECMWF diverse 117 profile set) but with same LbL model computed transmittances
  - » Gives estimate of inherent model accuracy of trasmittances and TOA radiances
- Fast model comparisons (e.g. Garand et al 2001 for HIRS and Saunders et. al. for AIRS) radiances and jacobians
  - » Gives performance of model compared to others
- Line-by-line model comparisons (e.g. ISSWG LIE)
  - » Gives estimate of underlying LbL model accuracy
- Comparisons with real satellite data using NWP fields
  - » Allows validation over wide range of atmospheres
- Comparison with aircraft data (e.g. NAST-I)
  - » Limited sampling but can reduce uncertainties of variables



## RT model validation





#### 0.8 HIRS 2 0.4 0.0 -0.4-0.8wrt GENLN2 (K) HIRS 5 2.0 1.0 0.0 -1.0HIRS 9 15.0 10.0 5 0 0 0 HIRS 10 1.0 0.5 0.0 -0.5-1.0bias\standard deviation HIRS 11 1 5 -1.5-3.02.4 HIRS 12 1 6 08 -0.82.0 HIRS 15 1.0 0.0 -1.0OPTRAN GLATOVS MSCFAST SIMRAD FLBL HFFP MODTRAN RTTDV-5 OPTRANZ OP-GLN2 OP-LRTM MSCFA5T2 MALKMUS STREAMER SYNSATRA

## Garand fast model intercomparison for HIRS channels

Line by line models



## AIRS RT model Comparison

- Compare AIRS RT models
- Compute BTs for all 2378 channels for 52 profiles
- For some models compute jacobians for a selection of ~100 channels
- Document run times
- Complete by Sep 04



## AIRS RT model Comparison

Model	<b>Participant</b>	Direct	Jacobian
RTTOV-7	R. Saunders, METO	Yes	Yes
Optran	Y. Han, NESDIS	Yes	Yes
OSS	J-L. Moncet, AER	Yes	Yes
LBLRTM	J-L. Moncet, AER	Yes	Yes
RFM	N. Bormann, ECMWF	Yes	Yes
Gastropod	V. Sherlock, NIWA	Yes	Yes
ARTS	A. VEngeln, Bremen	Yes	No
SARTA	S. Hannon, UMBC	Yes	No
EOF	Xu Liu, NASA	?	?
4A	S. Heilliette, LMD	Yes	Yes
FLBL	D.S. Turner, MSC	Yes	Yes
<b>GENLN2</b>	Peter Rayer, METO	?	?
σ-IASI	C. Serio, Uni Bas	Yes	Yes
Hartcode	F. Miskolczi, NASA	Yes	No

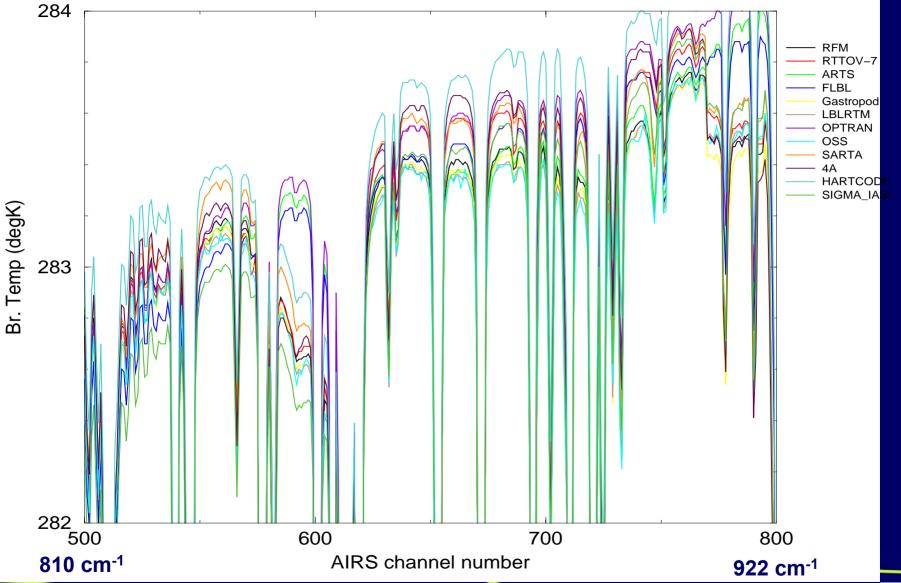


### **Initial Results**

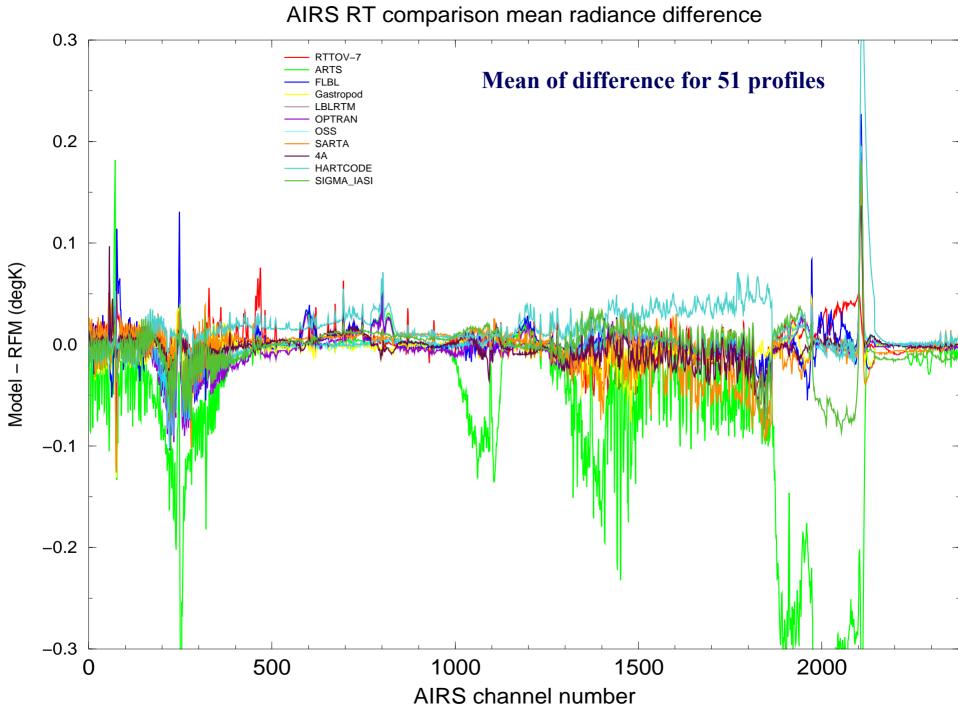
- ■To date have compared direct calculations for 12 models who have submitted results
- Used RFM as reference model (this may favour models based on GENLN2)
- Bias and sdev plots shown of differences for each AIRS channel for 51 diverse profiles



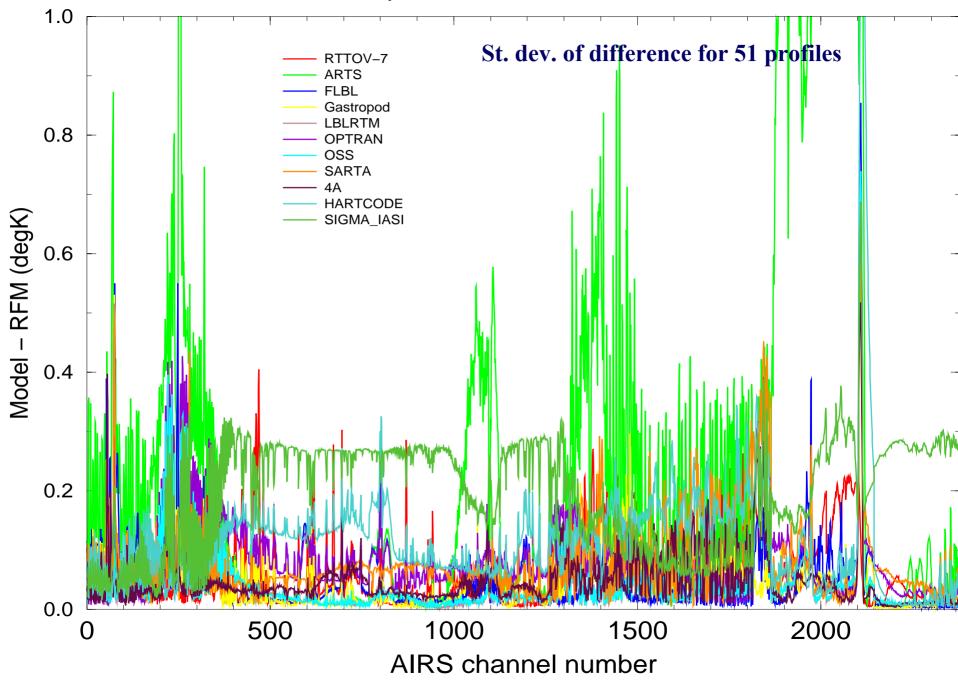
### AIRS RT model comparison

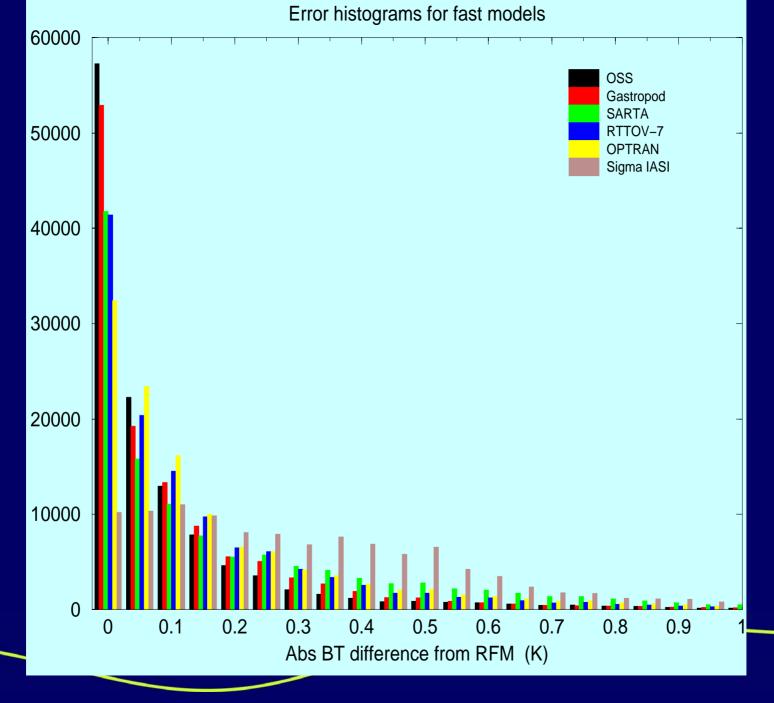






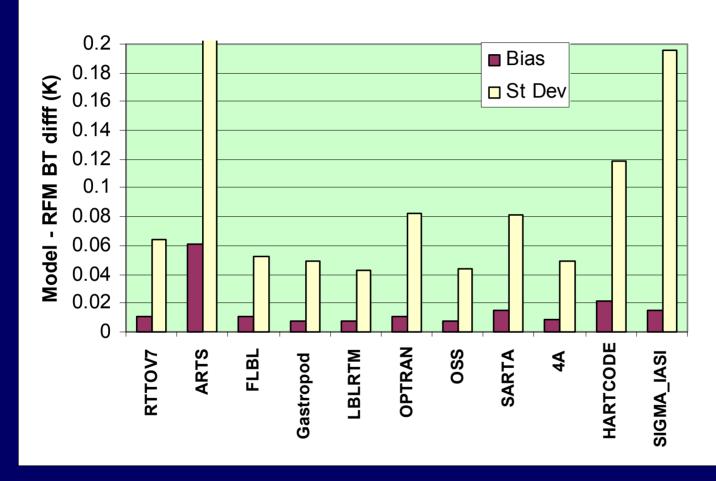
AIRS RT comparison st dev of radiance difference



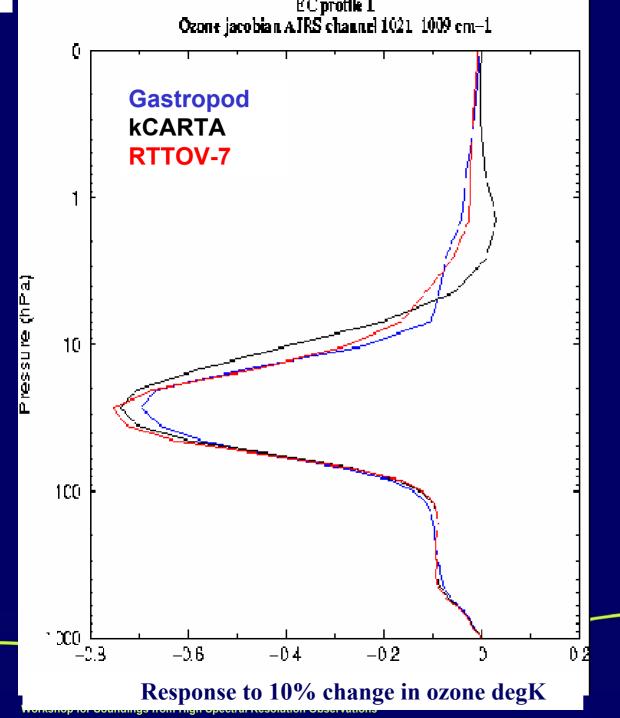




## Results averaged over all channels





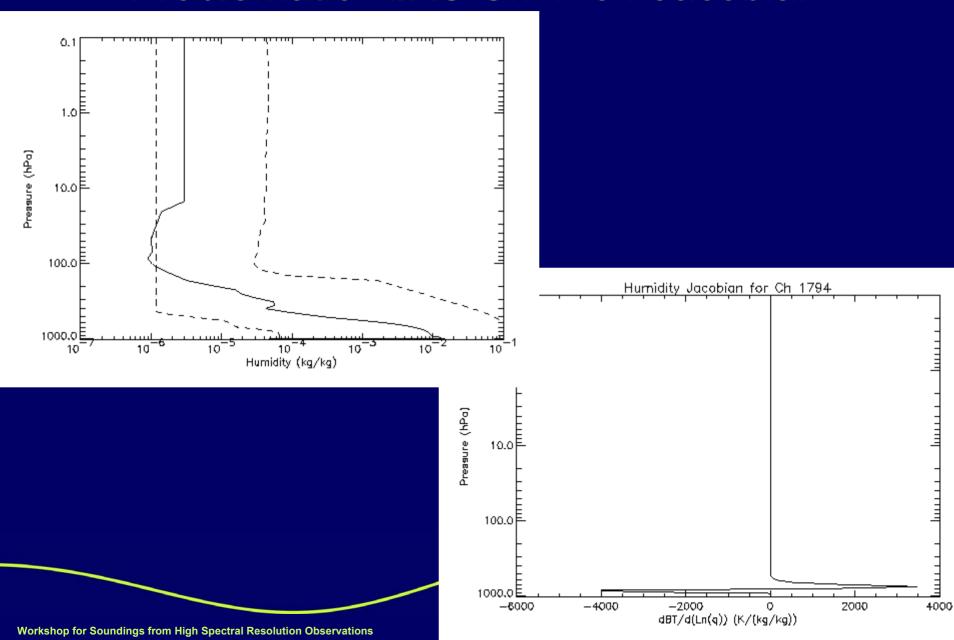


RTTOV-7 model validation for AIRS

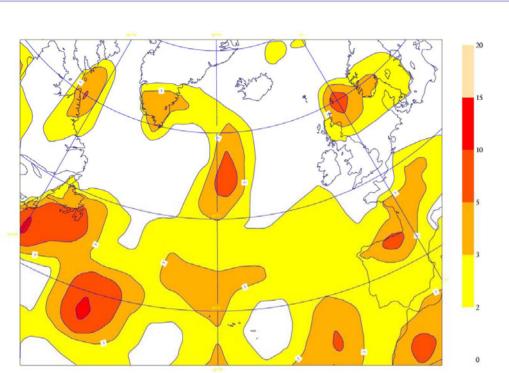
Ozone jacobian



## Problematic AIRS Ch 1794 Jacobian



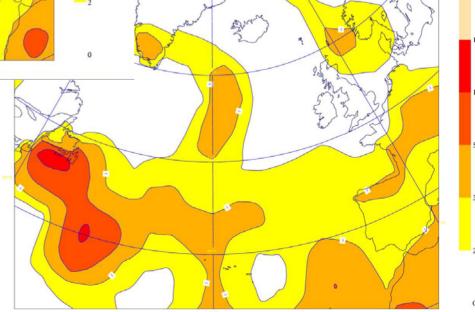
## **Validation within NWP model**



RTTOV-5

Model background error as HIRS-12 radiance

RTTOV-7



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## NWP Radiance Monitoring Observed minus Simulated

Continuous global view of data

0 0

- Good for spotting sudden changes in instruments
- Can compare with other satellites and in situ obs

But NWP model has errors: (LST, water vapour, ozone, clouds, stratosphere) so bias correction and cloud detection important and care in interpretation









- ► Home ► Research ► NWP ► Satellite Applications ► Infrared ► Advanced Sounders
- ► AIRS Monitoring ► Plots

 $NWP \mid Climate \mid Seasonal \ forecasting \mid Atmospheric \ processes \mid Oceanography \mid Projects \mid The \ stratosphere$ 

#### **AIRS Monitoring Plots**

#### **AIRS Monitoring Plots**

These plots are considered experimental. The Met Office accepts no responsibility for actions taken on the basis of these monitoring plots.

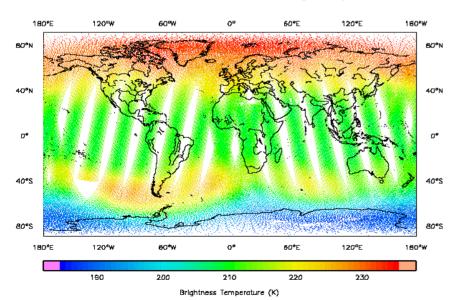
 Current:
 [57]
 First:
 [0]
 Last:
 [338]

Plot Type: Map of Raw BT 

Kip to:

Map of Raw BT

Observed BT for Channel 123 679.992 cm-1 (ivol = 56)



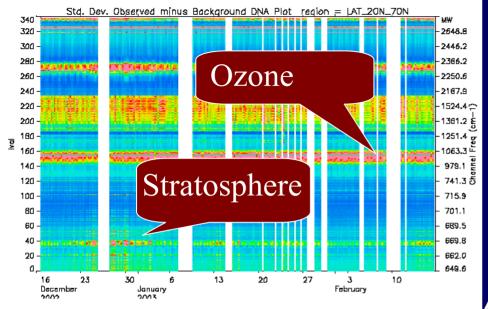
# Monitoring web page

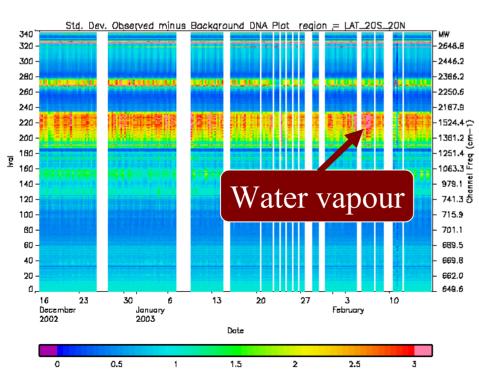
http://www.metoffice.com/research/nwp/satellite/infrared/sounders/airs/index.html

Userid: airspage

Passwd: &Graces

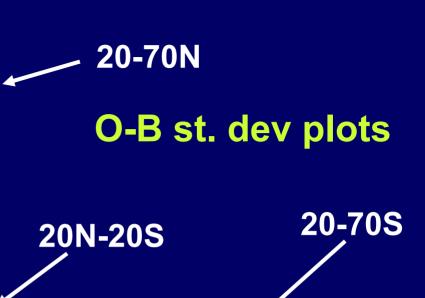


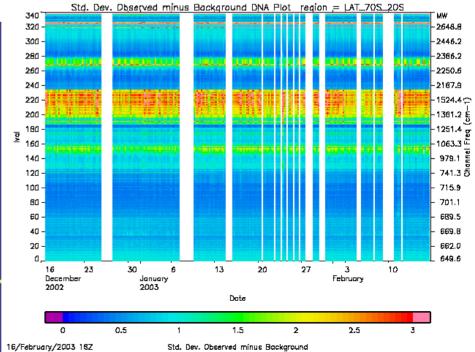




Std. Dev. Observed minus Background

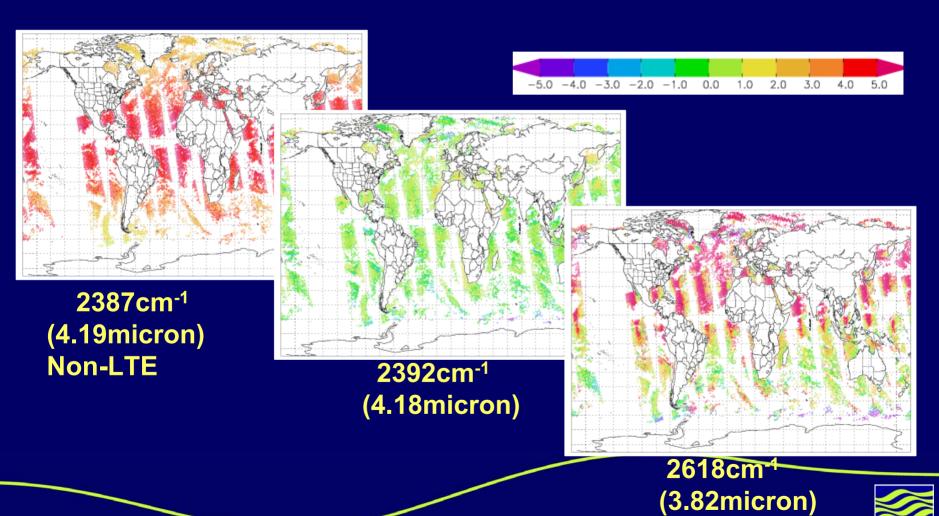
16/February/2003 18Z





## **O-B** difference

- Large positive bias in the SW-IR in the day-time due to Non LTE effect in upper sounding chs and sunglint in window



#### Assimilation of satellite radiances **Observation space** Observations O or V<sup>o</sup> Quality **Bias** Forecast observations B control O-B Ob correction (Forward modelled TBs) increments H(X)Adjoint of observation Observation operator H (Radiative transfer model + operator H map to observation space) Map back to model space **Profile** increments Adjusted model fields **Background NWP** forecast **Analysis Forecast NWP** model space



## Fast RT model in data assimilation

For variational assimilation want to minimise a cost function *J*:

$$J(X) = 0.5(y^{\circ} - H(X)) (O+F)^{-1} (y^{\circ} - H(X))^{T} + 0.5(X-X^{b}) B^{-1} (X-X^{b})^{T}$$

To minimise equation above, assuming the observations  $y^o$  to be linearly related to X then the minimum value for J(X) is when:

$$X = X^b + BH^{T} \cdot (H.B.H^T + O+F)^{-1} \cdot (y^o - H(X^b))$$

H is derivative of H wrt X often called jacobian matrix

$$\partial y = H(X_0).\partial X$$



## Issues for discussion

- Quantisation of training sets (levels, profiles,...)
- Good knowledge of instrument spectral responses
- Fast model methodology
- Is a unified model possible?
  - Infrared vs microwave can we use same model?
  - Limb path vs nadir can we use same model?
  - Fast models for NIR, visible radiances?
- Is underlying spectroscopy good enough?
- How do we treat aerosols, clouds and precip in fast models?



## Issues for discussion (2)

- Advanced sounders (>1000 chans) how can we use ?
- Improve robustness of jacobians for extreme profiles
- Allow for (O+F) correlations?
- Improve land/ice surface emissivity
- Need to trade off accuracy for speed





