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



From HIRS to IASI fast models

Spectrum of infrared radiation from atmosphere

HIRS 19 channels vs IASI 8461 channels



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 (cm ⁻¹)	649 –1135 1217–1613	Contiguous 645-2760	650 –1095 1210 –1750 2155 –2550
Unapodized spectral resolution (cm ⁻¹)	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

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

- 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

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)
- <u>Not</u> 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, O₃, CO₂, N₂O, CH₄, ...
 - 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. мт_ско, ско2.х)
- Line mixing and non-lte effects
- Well mixed gases to include
 (CO₂), CH₄, N₂O, CO, CFCs, N₂, O₂...
- Variable gases to include
 - H_2O , O_3 , (CO_2 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	For RTTOV-8
X _{j,1}	$sec(\theta)$	$sec^2(\theta)W_r^2(j)$	$sec(\theta) O_r(j)$	separate out water vapour line
X	$sec^{2}(\theta)$	$(sec(\theta)W_w(j))^2$	$\sqrt{sec(\theta)O_r(j)}$	and continuum +
X	$sec(\theta) T_r(j)$	$(sec(\theta) W_w(j))^4$	$sec(\theta) O_r(j) \delta T(j)$	more trace gases
X	$sec(\theta) T_r^2(j)$	$sec(\theta) W_r(j) \delta T(j)$	$(sec(\theta) O_r(j))^2$	
X j,5	$T_r(j)$	$\sqrt{sec(\theta)W_r(j)}$	$\sqrt{sec(\theta) O_r(j)} \delta T(j)$	
X j,6	$T_r^2(j)$	$\sqrt[4]{sec(\theta)W_r(j)}$	$sec(\theta) O_r(j)^2 O_w(j)$	
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	$sec(\theta) \frac{T_w(j)}{T_r(j)}$	$(sec(\theta)W_r(j))^3$	$sec(\theta) O_r(j) O_w(j)$	PTTOV 7
X j,9	$\sqrt{sec(\theta)}$	$(sec(\theta) W_r(j))^4$	$O_r(j) \operatorname{sec}(\theta) \sqrt{(O_w(j) \operatorname{sec}(\theta))}$	
X _{j,10}	$\sqrt{sec(\theta)} {}^4 \sqrt{T_w(j)}$	$sec(\theta) W_r(j) \delta T(j) \delta$	$ST(j)$ sec(θ) $O_w(j)$	Optical depth
X j,11	0	$(\sqrt{sec(\theta)W_r(j)})\delta I$	$F(j) \qquad (sec(\theta) O_w(j))^2$	predictors
X _{j,12}	0	$\frac{(sec(\theta)W_r(j))^2}{W_w}$	0	ΣK
X _{j,13}	0	$\frac{\sqrt{(\sec(\theta) W_r(j)} W_r}{W_w(j)}$	$\underbrace{(j)}_{0} \qquad \qquad$	$_{j-1} + \sum_{k=1}^{n} a_{i,j,k} X_{k,j}$
X	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	

Combining transmittances

For monochromatic calculations:

$$\tau_{total} = \tau_{mix} \times \tau_{wv} \times \tau_{oz}$$

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

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

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

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

Overview of PCA for fast RTM

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 \vec{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, H₂O and trace gases...)
- C_i 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





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

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

- 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

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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





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
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Model	Participant	Direct	Jacobian
RTTOV-7	R. Saunders, METO	Yes	Yes
Optran	Y. Han, NESDIS	Yes	Yes
ÓSS	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
GENLN2	Peter Rayer, METO	?	?
σ-IASI	C. Serio, Uni Bas	Yes	Yes
Hartcode	F. Miskolczi, NASA	Yes	No





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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





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° to be linearly related to X then the minimum value for J(X) is when:

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

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