Overview of fast model approaches and current issues

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Fast radiative transfer model for use in satellite data assimilation

The accurate computation of atmospheric transmittances/radiances is carried out using physical models based on first principles. These models are called *line-by-line models* (e.g. LBLRTM)

Line-by-line models, however, are too slow to be used operationally in e.g. NWP

The near real-time simulation of satellite data is carried out using *fast radiative transfer models*. These models are very computationally efficient and are able to reproduce line-by-line “exact” calculations very closely

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Fast RT models are generally based on LBL models

Many fast RT models have the capability of simulating radiances in a scattering atmosphere and many of them *cover a wide region of the electromagnetic spectrum from the microwave to the infrared to the visible*

The latter capability is of fundamental importance for NWP applications where the same fast model should ideally be used for all operational sensors including passive ones.

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There are several types of fast radiative transfer models, in use or under development, which are relevant to satellite data assimilation

The various models can be categorised into:

1) Narrow-band fast RT models on fixed pressure levels or on levels of fixed absorber amount
2) Library look-up based fast RT models
3) Neural network based fast RT models
4) Fast RT Models based on optimal sampling of absorption coefficients
5) Principal component based fast RT models
6) Physical models
7) Look-up table based fast RT models

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Narrow-band fast RT models on fixed pressure levels or on levels of fixed absorber amount

These fast RT models use regression coefficients derived from accurate LBL computations to compute atmospheric optical depths as a linear combination of profile dependent predictors that are usually functions of temperature, absorber amount, pressure and viewing angle

The regression coefficients are computed using a training set of typically less than 100 diverse atmospheric profiles chosen to represent the range of variations in temperature and absorber amount found in the atmosphere

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Narrow-band fast RT models on fixed pressure levels or on levels of fixed absorber amount

These models use the polychromatic form of the radiative transfer equation (i.e. they use channel averaged transmittances in the radiative transfer equation based on the assumption that this is equivalent to the convolution of the monochromatic radiances)

The polychromatic approximation is more than adequate for sensors with narrow spectral response functions. For sensors with broader channels, however, a manipulation of the transmittances (e.g. Planck function weighting) may be required for the polychromatic approximation to be accurate.

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Narrow-band fast RT models on fixed pressure levels or on levels of fixed absorber amount

The optical depths can be computed at fixed pressure levels as in the RTTOV (Matricardi et al., 2004) and SARTA (Strow et al., 2003) models.

The optical depths can be computed at levels of fixed absorber amount as in the OPTRAN model (McMillin et al., 1995).

The CRTM model (Weng et al., 2005) offers the possibility of using either the fixed pressure level or the fixed absorber amount approach

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Library look-up based fast RT models

These fast RT models are based on the library look-up approach (e.g. 3R (Rapid Radiance Recognition, Chédin et al, 1985). They make use of an extensive library of profiles and associated radiances created from a collocation dataset.

The fast model matches the input profile with one or a group of profiles in the library and then computes a radiance spectrum using the spectra associated to the matched profiles

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Neural network based fast RT models

Neural network based schemes have been developed for radiative transfer modelling applications (e.g. Chevallier et al., 2000). An artificial neural network realizes a nonlinear application from an input space (e.g. atmospheric parameters) to an output space (e.g. atmospheric radiances)

The development of a neural network based fast RT model requires the selection of learning datasets of atmospheric situations for all the variables that are included in the radiative computations

The accuracy of the scheme hinges on the statistical characteristics of these datasets. Several thousand atmospheric profiles are typically required for this purpose

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Neural network based fast RT models

The training of a neural network based fast model involves the accurate simulation of the radiances associated to each atmospheric situation. This task should be carried out using an accurate LBL model

Although the learning process is very time consuming, it should be noted that it has to be done only once unless the training has to be repeated due to a change in the vertical discretisation of the atmosphere

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Fast RT Models based on optimal sampling of absorption coefficients

The Optimal Spectral Sampling method (OSS) (Moncet et al., 2008) approximates spectrally integrated (i.e. polychromatic) radiances (or transmittances) with a weighted average of monochromatic radiances (or transmittances) calculated at a selected number of spectral points.

The OSS approach is an extension of the k-distribution technique to vertically inhomogeneous atmospheres. OSS is a fast method that allows to perform accurate radiative transfer computations for a wide range of applications

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Fast RT Models based on optimal sampling of absorption coefficients

The training of OSS involves LBL computations carried out for a set of diverse atmospheric situations.

The OSS method can be easily extended to scattering atmospheres and can be in principle applied to any linear transformation of the spectral space (e.g. principal components).

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Principal component (PC) based fast RT models

PC based fast models parameterise the PC scores of the radiance spectrum. The PC scores have much smaller dimensions as compared to the number of channels. This optimizations results in significant computational savings and in a very accurate simulation of the radiances

The training of PC based fast RT models requires the computation of a large database of LBL spectra for a diverse set of atmospheric and surface situations. The training spectra are assembled in a large matrix from which the PCs of the radiance spectra are computed by applying singular value decomposition to the radiance matrix

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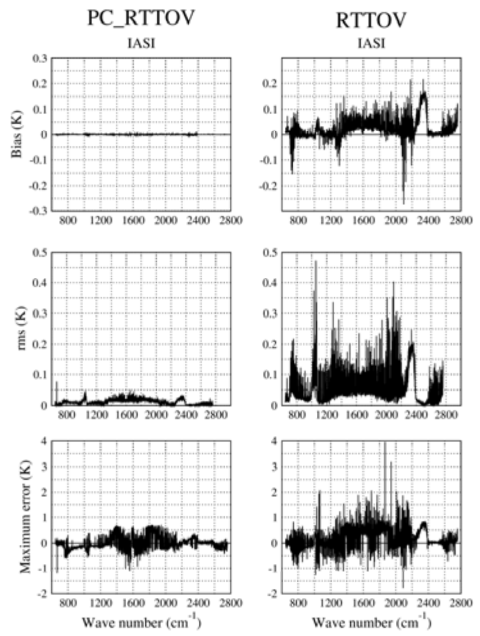
Principal component (PC) based fast RT models

Whilst the principal components are fixed, their scores (weights) vary from profile to profile and they can be predicted using a linear regression scheme where they are expressed as a linear combination of profile-dependent predictors

In PCRTM (Liu et al., 2006) and HT-FRTC (Havemann et al., 2014) the predictors are monochromatic radiances at selected frequencies

In PC-RTTOV (Matricardi, 2010) the predictors are polychromatic (channel) radiances calculated by RTTOV



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Principal component (PC) based fast RT models

The linear relationship between radiance predictors and principal component scores is established by a regression on the training data set

It should be noted that while monochromatic predictors are comparatively straight-forward to calculate, even if many trace gases are involved, the calculation of polychromatic predictors requires a more complicated and more time-consuming transmittance prediction system

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Principal component (PC) based fast RT models

In the context of PC based fast models it is possible to generate sensor-independent principal components at full line-by-line resolution allowing flexible changes regarding the specification of the instrument response function

- PC based fast RT models have been employed in the retrieval of atmospheric and surface information (e.g. HT-FRTC ,Thelen et al. 2009).

- In the context of operational NWP data assimilation, PC-RTTOV has been successfully used at ECMWF for the testing of the direct 4D-Var assimilation of principal components derived from IASI fully clear spectra (Matricardi and McNally, 2014)

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Physical fast radiative transfer models

This approach *averages the spectroscopic parameters* for each channel and uses these to compute layer optical depths.

Compared to fast RT models currently used in data assimilation, this approach offer several advantages:

1) More accurate computations for some gases
2) Any vertical co-ordinate grid can be used
3) It is easy to modify if the spectroscopic parameters change

Physical fast RT models, however, are a factor 2-5 slower which is significant for assimilation purposes

Priorities for future recearch

Spectroscopic parameters

1) It should be assessed if there is any requirement regarding the precision of the spectroscopic parameters

2) Using the synergy between the IR and the UV/Vis some inconsistencies have been observed in the retrieval of ozone profiles which could attributed to an inconsistency of the precision of the spectroscopic parameters between the two spectral ranges. Inconsistency problems have also been observed for SO_2.

3) Promote research in to spectroscopy of higher frequency microwave channels up to 664GHz.

4) Line shapes of water vapour broadening for trace gases need improvement

Priorities for future recearch

Lineby-line models

1) There are concerns that line-by-line models are not flexible enough to accommodate the use of line parameters from alternative databases

2) Although the semi-empirical MTK_CKD continuum model is perhaps adequate for NWP applications, there is still the need for a physically based representation of the continuum absorption which should eventually be implemented in state-of-the-art LBL models

3) Further research is needed into the modelling of line mixing processes for CO_2, CH_4, N_2O and to a lesser extent water vapour. This is especially true for the 4µm absorption band of CO_2.

4) The effects of pressure and Doppler line broadening should be modelled using a better representation of the line shape than the Voigt profile. Proposed replacements to the Voigt profile will require different broadening coefficients for all the molecules and consequently the need for significant updates to LBL models

Priorities for future recearch

Scattering models

1) The validation of the scattering approximations used in fast RTM models is of crucial importance for a successful operational use of fast RTM in scattering atmospheres

2) The effects of three-dimensional cloud structures should be studied. Simplified methods like the one used in RTTOV have been developed to deal with inhomogeneous cloud fields. However, they can only provide a gross approximation of the inhomogeneity observed by a satellite borne instrument.

3) To allow full synergy, there is a need for a consistent treatment of scattering across the spectrum (e.g. in the treatment of non-spherical ice habits).

4) Do we continue investing resources into the development of fast parameterisations/approximations of scattering for NWP or we can now afford the use of more complex (and slower) schemes?

Priorities for future recearch

Models for the microphysical and optical properties of scattering particles

1) There is a need to represent in a consistent way the optical and scattering properties of across the spectrum

2) Efforts on the calculation of optical properties should continue focusing on an efficient and accurate solution of the problem for non-spherical particles

3) The representation of the optical properties of an ensemble of scattering particles of different sizes and different habits is still an outstanding issue and more research is needed into the characterisation of the size distributions. This is especially true for ice particles for which a variety of different habits has been observed.

4) There is an urgent need for larger public datasets of aerosol refractive indices and their variability. These datasets should also include information on measured size distributions and their natural variability. This is especially important for mineral aerosols but also for secondary aerosols (sulphuric acid, ammonium salts, boundary layer PM).

Priorities for future recearch

Emissivity models

1) Unified physical model of hemispherical emissivity/BDRF/Sun-glint functions?

2) How do we characterise the statistical properties of the sea surface? Should we select a reference wave model?

3) There is also a need to understand how complex mixtures of surfaces inhomogeneity is represented

4) Should we develop and maintain global atlas products of emissivity?. It is also important that atlases keep track with land use changes.

Priorities for future recearch

Datasets of atmospheric profiles and validation of RT models

1) Continued requirement for validation campaigns to assess uncertainties in the RTM

2) Greater understanding of the relative importance of the uncertainties in the RT modelling e.g. how large the uncertainties are in the spectroscopic data and how they impact the radiances

3) Profile datasets should include more gas species. In addition, there is a requirement for datasets that include state vectors for clouds and aerosols

Priorities for future recearch

Fast models for NLTE

1) Fast NLTE models require a training dataset of atmospheric profiles. How good are these profiles in representing the atmospheric variability in the upper stratosphere/mesosphere?

2) The current training of fast NLTE models does not adequately represent the ozone variability in the mesosphere (i.e. the occurrence of mesospheric ozone tertiary maxima at high latitudes during winter).

3) The training of fast NLTE models require the computation of a database of vibrational temperatures for a large number of CO_2 vibrational states.