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The Havemann-Taylor Fast Radiative Transfer Code (HT-FRTC): A multipurpose code based on principal components

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ABSTRACT

The HT-FRTC can be used across the electromagnetic spectrum from the microwave through to the ultraviolet to calculate transmittance, radiance and flux spectra, which are represented by their principal components. The code uses monochromatic calculations at a small number of frequencies, which are selected by k-means clustering, to predict the principal component scores. It has been found that kernel regression yields more robust predictions than a linear regression. The principal components cover the spectrum at a very high spectral resolution, similar to that of conventional line-by-line models such that the individual spectral lines are resolved. This approach allows very fast line-by-line-like, hyperspectral and broadband simulations for satellite-based, airborne and ground-based sensors. The principal components are derived during a code training phase from monochromatic simulations for a diverse set of atmospheres and surfaces. They are sensor independent and no extra training is required for additional sensors. The HT-FRTC has been trained with all of the trace gases in the HIgh-resolution TRANsmission molecular absorption database (HITRAN) and on a large variety of surface emissivity/reflectance spectra. It can be run for any Lambertian or specular surface. The HT-FRTC is a plane-parallel one-dimensional model but some effects of the Earth's sphericity are accounted for. Solar, lunar and cosmic microwave background sources have been included. Scattering by frozen and liquid cloud, precipitation particles and twenty different aerosol species has been included, as well as Rayleigh scattering which is significant in the short-wave. The scattering phase function can be fully accounted for by an integrated monochromatic version of the Edwards-Slingo spherical harmonics radiation code or approximately by a modification to the extinction (Chou scaling).

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1. Introduction

During the last decade the number of Earth observing hyperspectral radiometers deployed in space has rapidly increased. Instruments on polar orbiting satellite platforms like the Atmospheric Infrared Sounder (AIRS) on Aqua [1], the Infrared Atmospheric Sounding Interferometer (IASI) on the Meteorlogical Operational Satellites MetOp-A and MetOp-B [2,3] and the Cross-track Infrared Sounder (CrIS) on the Suomi National Polar-orbiting Partnership (Suomi NPP) [4,5] are covering the thermal and mid-infrared while Hyperion on the Earth Observer (EO)-1 operates as a hyperspectral imager in the near-infrared and short-wave [6]. Future instruments like IASI Next Generation (IASI-NG) [7] will have twice the spectral resolution of IASI and the Meteosat Third Generation InfraRed Sounding (MTG-IRS) [8] will be a hyperspectral instrument on a geostationary platform generating significantly increased data volumes.

The assimiliation of these hyperspectral satellite data into Numerical Weather Prediction (NWP) systems requires fast radiative transfer models that can simulate hyperspectral spectra for given atmospheric and surface conditions. For conventional fast models like the Radiative Transfer for TOVS (RTTOV; TOVS stands for TIROS Operational Vertical Sounder and TIROS for Television Infrared Observation Satellite), the computational time increases proportionally to the number of channels that are assimilated [3,9]. Some of the channels of hyperspectral sounders like IASI are highly correlated with similar weighting functions. The addition of such channels in the assimilation is nevertheless beneficial as it has the effect of reducing the noise level of the combined measurement compared to that of a single channel.

The use of principal components [10] of the radiance spectra rather than the radiances themselves is one way to dramatically speed up the calculations while conserving the information content of the full spectrum. During a code training phase a diverse

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set of atmospheric and surface conditions is used to generate an equally diverse set of radiance spectra from which the principal components are generated. While the principal components themselves are fixed spectra, their scores (weights) change as atmospheric and surface conditions change. Different predictors may be used for these PC scores. In the case of the Principal Component-based Radiative Transfer Model (PCRTM) [11,12] and the HT-FRTC [13], a few hundred monochromatic radiances are used as predictors. The HT-FRTC uses a k-means clustering algorithm during the training stage for the selection of the frequencies at which these radiance calculations are required. There is also the Principal Component based RTTOV (PC-RTTOV) [14], which uses the polychromatic (i.e. channel) radiances produced by RTTOV to predict the principal component scores. The polychromatic radiance calculation in RTTOV requires a transmittance prediction scheme [9], which makes this approach computationally more demanding compared to the models that are based purely on monochromatic radiances [11,13].

While the HT-FRTC was initially developed only for clear-sky atmospheres [13], the next stage was to include a monochromatic full scattering capability with the view to treat aerosols and clouds as well as Rayleigh scattering in the short-wave. The scattering calculations were initially done by calling the DIScrete Ordinate Radiative Transfer (DISORT) model [15,16] as a module using very narrow spectral bands. This was later supplemented by a monochromatic version of the Edwards-Slingo code [17,18], which treats scattering fully. The capability of the HT-FRTC to simulate scattering atmospheres was applied to hyperspectral radiance observations made by the Airborne Research Interferometer Evaluation System (ARIES) instrument [19] on board the Met Office BAe146 aircraft affected by volcanic ash from the Eyjafjallajoekull eruption [20]. The code has also been used to simulate IASI observations of sulphur dioxide from volcanic eruptions [21]. For some years now the HT-FRTC has been used operationally as part of the Met Office NEON Electro-Optic Infra-Red Tactical Decision Aid (TDA) [22]. Simulations with HT-FRTC have been included in a recent radiative transfer model evaluation study which focused on the simulation of cloudy AIRS observations [23].

Another application of the HT-FRTC has been as part of one dimensional variational (1D-Var) retrievals of atmospheric and surface parameters [24] performed solely in principal component space. Among these were retrievals of surface emissivity (simultaneously with vertical profiles of temperature and water vapour) from ARIES measurements on board the Met Office British Aerospace BAe146 aircraft [25]. In these retrievals the surface emissivities were represented by a set of principal components just like the radiances. The retrieval of surface properties has been extended into the short-wave, where surface reflectance spectra were obtained together with atmospheric profiles from hyperspectral images taken by Hyperion [26]. The HT-FRTC has also been used in retrievals from ARIES measurements in the presence of cirrus clouds, where the radiance residuals from the retrievals were used to investigate the spectral consistency of the cirrus optical properties [27]. Simultaneous retrievals of cirrus cloud properties and profiles of temperature and water vapour were performed, the latter being compared to predictions from the Met Office NWP model [28]. The retrieved parameters of the cirrus cloud in [27] and [28] were the cloud top pressure, the cloud thickness, the cloud ice water content and the horizontal cloud fraction. Effective size was not one of the parameters, as the cirrus optical properties were parameterized solely as a function of cloud temperature and cloud ice water content [27]. The cloud top and bottom were allowed to move by small increments independent of the atmospheric layer structure. In other words, the layers containing the cloud top and the cloud bottom tended to be only fractionally covered by cloud in the vertical. The clouds typically extended over several adjacent layers.

Recently the HT-FRTC has been redesigned. The most significant change relates to the principal components themselves. Like in the case of PCRTM [11] and PC-RTTOV [14], the previous version of HT-FRTC [13] defined a separate set of principal components for the spectra of every instrument that needed to be simulated. This meant that the code had to be retrained for a new instrument and even for a new channel selection or for small changes in the definition of the spectral characteristics of the instrument channels. In the new version of the HT-FRTC, the principal components are derived at the very high resolution typically found in line-by-line models. This offers immense practical advantages as any number of instruments can now be simulated without the need to retrain the code. Retraining is only required when the spectroscopy or the radiative transfer algorithm is updated. Fast calculations at any spectral resolution (i.e line-by-line-like, hyperspectral or broadband) are all possible with the same set of principal components. In the next section (Section 2.), a detailed description of the new sensor-agnostic version of the HT-FRTC will be given. Code validation results which quantify its accuracy are presented in Section 3. and a selection of results for different applications have been assembled in Section 4. Following these, some conclusions are drawn in Section 5.

2. The HT-FRTC

The HT-FRTC contains as a central part a complete, monochromatic radiative transfer code. It can be run at a very high spectral resolution producing output like that of a line-by-line code. This is the way the HT-FRTC is run during the code training stage. The same monochromatic code, albeit only at a small set of selected frequencies, is also called when the fast code is run. The monochromatic code will be discussed in the following Section 2.1, followed by a Section 2.2 on the specifics of the training code, a separate Section 2.3 on the subject of the clustering code that is used to find a frequency selection for the fast code. This is followed by a Section 2.4 on the specifics of the fast code for simulations at very high line-by-line-like, hyperspectral and broadband resolutions. The final Section 2.5 contains a discussion of the computational timings and demonstrates the speed-up the fast code makes possible when compared to full monochromatic calculations for both clear-sky and scattering atmospheres. It also details what computational resources are required for the individual tasks that are required during the code training.

2.1. The monochromatic code

The HT-FRTC allows monochromatic calculations across the electromagnetic spectrum from $3\,MHz$ (i.e. $10^{-4}\,\mathrm{cm}^{-1}$ in wavenumbers or 100 m in wavelength) to 1500 THz (i.e. $50,000\,\mathrm{cm}^{-1}$ or $0.2\,\mu$ m). The code can be run at any spectral resolution and allows an arbitrary frequency grid for the monochromatic calculations, which does not need to be equidistant. For accurate results the individual spectral lines need to be sufficiently resolved. In general the width of the spectral lines is due to pressure and Doppler broadening. At very low atmospheric pressures at high altitudes only the Doppler broadening is significant. To ensure that the thinnest lines are adequately sampled, a relative spacing of 3×10^{-7} is used [29]. This is the ratio of the frequency spacing to the actual frequency and the same holds in wavenumbers and wavelengths. For instance, at 1000 cm^{-1} (10 µm) the spacing between two adjacent spectral grid points is 3×10^{-4} cm^{-1} (3 p.m.). To cover the spectral range of infrared hyperspectral instruments between 600 cm^{-1} and 3000 cm^{-1} at total of 6 million grid points

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