LIDORT family of Radiative Transfer Models Applications to the TEMPO Project

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Outline of Talk

- LIDORT Family Overview
  - LIDORT/VLIDORT main codes
  - LIDORT-RRS summary
  - FO (single scatter), 2STREAM and 2OS codes
  - Linearized Mie and T-matrix codes
- Accelerated Radiative Transfer: PCA methods
- Applications of RT models to TEMPO (Brief)
  - The GeoCape tool as template
  - TEMPO retrievals overview

LIDORT Family Overview (1): LIDORT/VLIDORT

- LIDORT and VLIDORT are multiple-scattering discrete ordinate radiative transfer codes in stratified atmospheres. Solution of RTE by Eigenvalue methods (both), Green's functions (LIDORT), substitution methods (VLIDORT).
- LIDORT is scalar (no polarization); generates radiance I
- VLIDORT is vector (with polarization); generates Stokes 4-vector [I,Q,U,V] → fully compatible in every respect with the scalar LIDORT code.
- Diffuse (multiple) scattering in plane-parallel medium, but solar attenuation (before scattering) treated spherically → the pseudo-spherical approximation.
- Single scattering can be treated precisely (solar and viewing paths both treated for a spherically curved atmosphere).
- Output is available for downwelling and upwelling fields anywhere in the atmosphere (level boundaries, partial layers), for various combinations of solar and viewing geometries.
- Mean-value output is available (fluxes, actinic fluxes).

LIDORT Family Overview (2): LIDORT/VLIDORT

- Both codes have atmospheric and surface *thermal emission* treatments, based on ingestion of Planck functions specified at surface and layer boundaries.
- Both codes have *BRDF supplements*, which are separate modules providing necessary BRDF inputs to the main code.
- There are also "*surface leaving*" supplements, providing surface-leaving radiance source (applications so far, mainly for fluorescence)
- Both codes are fully "Linearized", that is, they are able to simultaneously generate any number of analytically derived Jacobians (weighting functions, sensitivity functions, partial derivatives of I,Q,U,V) with respect to profile quantities (e.g. O3) or total-atmosphere "column" quantities (e.q. total AOD, total O3), or surface properties(e.g. albedo, glitter wind speed).
- LIDORT first developed in 1999 at SAO, VLIDORT from 2004 on. F77.
- Currently Versions 3.6 (LIDORT), 2.6 (VLIDORT). F90 now.
- User Guides for both codes. On the web at www.rtslidort.com
- Codes in public domain. Available from RT SOLUTIONS (rtsolutions@verizon.net)

LIDORT Family Overview (3): LIDORT-RRS

- LIDORT-RRS is a scalar LIDORT-based multiple-scattering code which includes rotational-Raman scattering by air molecules. Photons are scattered inelastically just once; elastic scattering to all orders.
- Completely compatible with LIDORT when RRS is turned off.
- All major LIDORT-style options are available (precise single scatter calculations, pseudo-spherical approximation, general output options…)
- Code operates in "binning" and "monochromatic" modes, depending on usage of input solar spectrum. Much slower than regular LIDORT code.
- Developed from 2003 onwards; Linearized in 2011; vector code currently under construction. F90 now. This is a research code.
- Important for simulating accurately the "filling-in" of Fraunhofer and telluric (absorption) features – the Ring effect. Useful for LUTs of filling factors and offline closed-loop testing of semi-empirical Ring algorithms

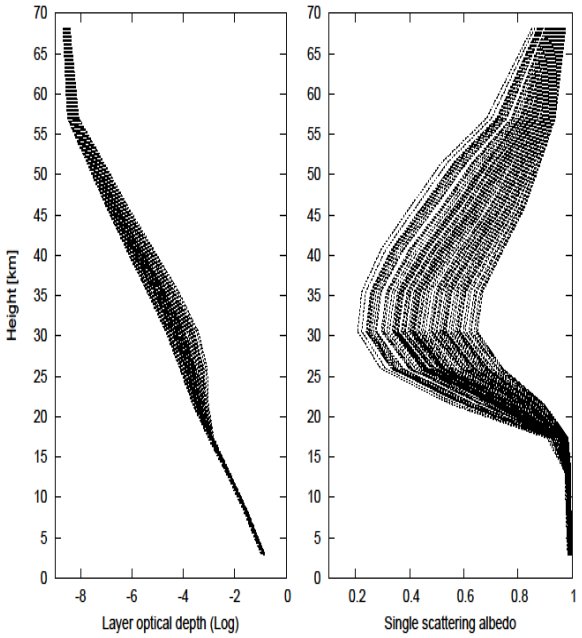
LIDORT Family Overview (4): FO, 2STREAM, 2OS codes

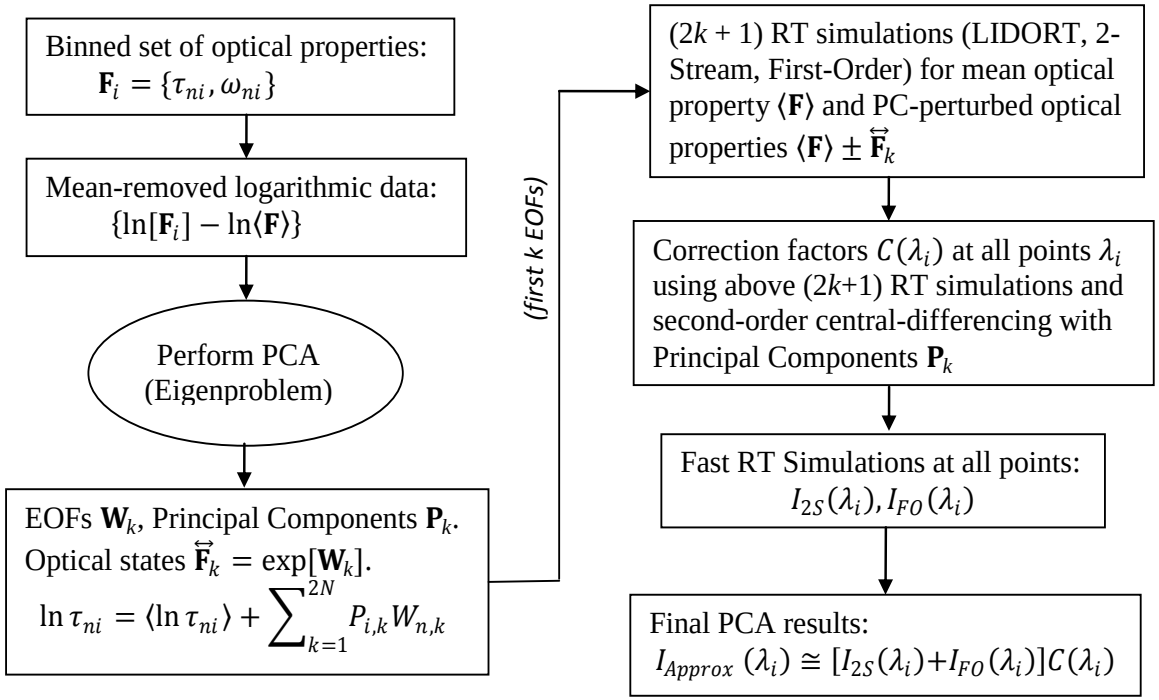
- FO (First-order) codes: stand-alone fast and accurate single scattering codes (scalar/vector/RRS). Fully linearized.
- FO codes have thermal emission, BRDFs → nearly all the same facilities as the parent LIDORT codes. LIDORT/VLIDORT/RRS compatible.
- FO Example: Use along with VLIDORT as an external alternative to VLIDORT's internal SS codes (which are not stand-alone). Then, VLIDORT runs in MS mode only. Eventual uses inside VLIDORT and LIDORT (under construction).
- 2STREAM is a fast multiple-scatter-only scalar code for TOA upwelling and BOA downwelling output. Just 2 discrete ordinates, fully linearized, pseudo-spherical, thermal emission, BRDFs. Spurr and Natraj (2011).
- 2STREAM designed for use in fast-performance RT modeling, in conjunction with LIDORT and the FO scalar codes. → example to follow….
- 2OS is a second order of scattering code developed originally for the OCO algorithm (Natraj and Spurr, 2007). Fast model to generate intensity corrections and polarization estimates, to be used in conjunction with LIDORT.
- 2OS originally TOA upwelling only + profile Jacobians. Currently undergoing extensions to other linearization outputs + wider range of output options.

LIDORT Family Overview (5): Linearized Mie and T-matrix Codes

- Mie code linearized 2004, based on 1980s Meerhoff code (Netherlands). Spherical particles.
- T-matrix code linearized 2011, based on 1990s GISS code (Mishchenko et al.,). Spheroids, Cylinders, Chebyshev particles. R. Spurr, J. Wang, J. Zeng. M. Mishchenko, JQSRT **113** (2012)
- Codes generate Optical Properties Ψ = { Extinction and scattering cross-sections, generalized spherical-function expansion coefficients, scattering (F) matrices }.
- Monochromatic or polydisperse. Usual choices of PSD (lognormal, gamma, etc.). Full Bimodal. F90 codes in public domain, with User Guides.
- Linearization: Jacobians (analytical derivatives) of Ψ w.r.t microphysical aerosol properties: components of refractive index, shape factor (T-matrix), and PSD parameters.
- Use linearized Mie/Tmatrix packages working together with linearized vector RT models such as VLIDORT. Such "combination" tools are finding use in OSSEs – Large-scale simulation experiments examining sensitivity and performance issues.
- More convenient (and arguably more fundamental) to characterize atmospheric aerosols in terms of profiles characterized by a small number of parameters (e.g. Exponential decay, Gaussians), and a small number of microphysical optical properties.
- Alternative to possible over-specification of macroscopic aerosol properties (profiles of aerosol optical thickness, single scattering albedo, F-matrix expansion coefficients).
- Application to aerosols (over the oceans) retrieved from GOME-2 using broad-band polarization measurements [Hasekamp et al., 2005]; early use of linearized Mie code with vector RT. Butz et al (2009) study for OCO, methodology now incorporated in OCO-2 algorithm.

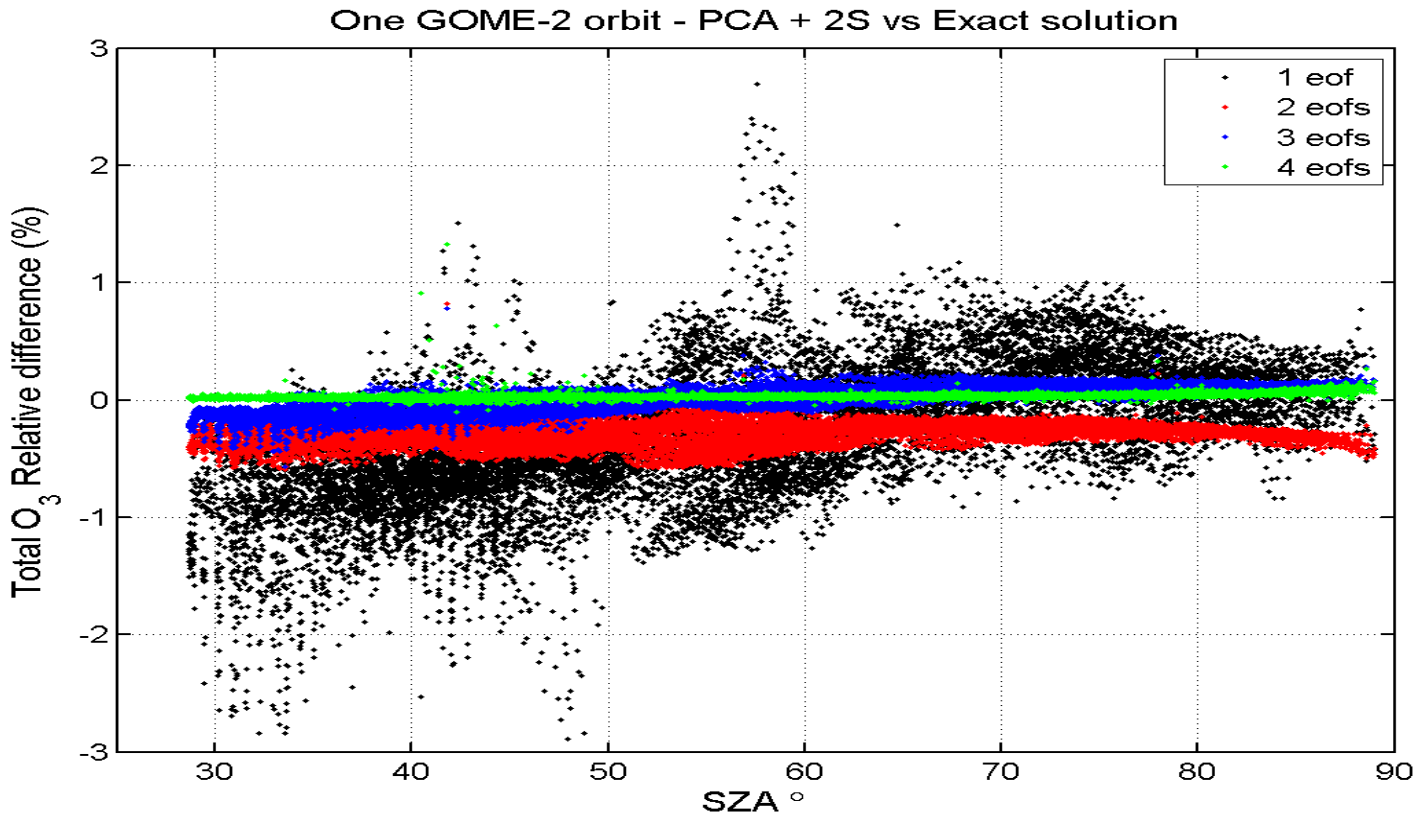
Accelerated RT using PCA (1)





- Set of optical properties (e.g., optical depths + single scattering albedos, 325-335 nm Rayleigh + O3 absorption).
- Perform PCA on mean-removed data set: → Use small set of "dominant" profiles (Mean+EOFs) as input to LIDORT , 2Stream → Use Principal Components to get correction factors, Use 2S and FO to get approximate radiances. Combine to restore radiance field.

Accelerated RT using PCA (2)



- Relative differences in retrieved total ozone for one GOME-2 orbit; PCA calculations using 1, 2, 3, 4 EOFs. Orbital processing times of 7795 seconds (exact), 1873s, 2035s, 2227s, 2532s; performance enhancements 4.16, 3.83, 3.50 and 3.08.
- March 2013 (ESA CCI project for ozone); entire GOME, GOME-2 and SCIAMACHY records to date, processed in ~3 weeks using this PCA speed-up.
- Spurr et al., JQSRT, 2013. Lerot et al., 2013 to appear.

Applications to TEMPO (1): The Geocape Tool

- GeoCape Tool is hyperspectral Forward + Inverse model simulation tool for sensitivity studies for American geostationary instrument.
- Forward-model part is based on VLIDORT, but also contains linearized Mie code, and FO code for external single scatter calculation (some later versions).
- Two main threads (spectral regions), UV/Vis +Thermal/Crossover.
- Natraj et al., *Atmos. Env.*, **45** (2011) : "Multispectral sensitivity studies for the retrieval of tropospheric and lowermost tropospheric ozone from simulated clear sky GEO-CAPE measurements."
- Constructed 2009-2010 as part of the initial GeoCape Studies project.
- Variants of the GEOCAPE Tool are now in use in several projects in the USA, Europe and East Asia. These variants are being applied not only to algorithm development studies for present and future GEO Instruments, but also for OSSEs investigating instrument synergies with LEO instruments.

Applications to TEMPO (2): Retrievals

- TEMPO: 290-690 nm, ~2K spectral points, 1250 E-W scans, 2.0x4.5 km^2 pixel at 36.5N, 100W. Geostationary North America.
- Trace gases: O3, NO2, SO2, H2CO, C2H2O2, H2O. O3 Profiles
- O2-O2, O2 (B and γ), Aerosol, Clouds, UVB radiation
- Lot of heritage and experience with these retrievals, with American instruments (OMI, MODIS, OMPS….) and European projects (GOME/GOME-2, SCIAMACHY)
- Talks to follow this afternoon: status/plans on retrievals.
- In several cases, forward modeling radiative transfer done using one (or more) of LIDORT family of models.
- Lots of data with new generation of atmospheric chemistry instruments (LEO and GEO) having much higher spatial resolution (e.g. TROPOMI vs. OMI).
- Accelerated RT will be important, e.g. PCA applied to LIDORT and 2Stream (fast scalar RT), or PCA applied to VLIDORT and 2OS (fast polarization correction), or fine/coarse layer distinctions (SS versus MS modeling)…..