

FASCODE for the Environment (FASE)

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Abstract

The Optical Physics Division of the Phillips Laboratory, with support from the U.S. Department of Energy (DOE) Atmospheric Radiation Measurement (ARM) Program, is developing a state-of-the-art line-by-line atmospheric radiative transfer model as the successor to FASCODE. The goal of this project is to create a computationally efficient model which contains the most up-to-date atmospheric physics. The new model, known as FASCODE for the Environment, or "FASE", will combine the best features of FASCODE and LBLRTM, the DOE's standard radiative transfer model. FASE will also contain new features such as new cross-sections for heavy molecules, an improved solar irradiance model, and improvements to the Schumann-Runge bands and continuum. The code will be optimized for vectorized and/or parallel processing, put under configuration control for easy maintenance, and structured into separate modules for each function: atmospheric profiles, layer optical properties, radiative transfer, multiple-scattering, etc. This modular structure will allow for increased flexibility and easy customization of the code for specialized applications, such as a forward model for iterative inversion algorithms. Ease-of-use will be enhanced with improved input control structures and documentation to accommodate the needs of novice and advanced users. This paper addresses changes which have been made to FASCODE and LBLRTM to create FASE, and gives an overview of the modular structure and its capabilities.

Introduction

The goal of the FASCODE for the Environment (FASE) program is to create an atmospheric radiance and transmittance model which is user-friendly and contains the latest atmospheric physics. The prime focus of the

program is to make available to the atmospheric spectroscopy community the results of on-going work sponsored by the U.S. Department of Energy (DOE), while incorporating the results of continuing research and development at the Air Force Phillips Laboratory. In addition, advances from the wider radiative transfer community will be incorporated where appropriate within program constraints and resources.

FASE has been developed by combining features from the line-by-line radiative transfer codes of the Air Force Phillips Laboratory (FASCODE) (Anderson et al. 1994) and the Department of Energy (LBLRTM) (Clough 1993). Both of these models were derived from FASCOD3 which was based on FASCOD1B, a four-function line-by-line code developed by Clough and Kneizys (Clough and Kneizys 1979). Our basic approach to developing FASE is severalfold: 1) to modify the overall program structure of FASCODE/LBLRTM so as to improve the flexibility and maintainability of the code without significant recoding, 2) to incorporate a number of coding improvements (also to benefit the flexibility and maintainability), 3) to improve the user interface and access to individual portions of the code, and 4) to add new modules which incorporate updated physics and improved features. These tasks have been identified as those which would be the most beneficial to current users of the code. For those that use the code as a "blackbox" by supplying the appropriate input and examining the output, FASE will appear identical to FASCODE/LBLRTM. However, for users who wish to modify the code or incorporate it within other software, FASE will be a much easier code with which to work.

The key features of FASE are shown in Table 1. Items of scientific interest include a more accurate algorithm for the Voigt profile, updated non-local thermodynamic equilibrium (NLTE) routines, a line rejection flag to signal

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Table 1. Key features of FASE.

Science Improvements	Coding Improvements
Improved Voigt Algorithm	Parameterization of Array Sizes
Updated NLTE Routines	Output in NCAR Graphics Format
Line Rejection Flag	Coded for Vectorized Computers
Schumann-Runge Bands and Continuum Programs	Output Formatted for Multiple-Scattering
Solar Spectrum Model	Embedded FFT Scanning Functions
Improved Hartley-Huggins and Chappuis Bands	Optional Fixed DV Output 2020 cm ⁻¹ Spectral Region (max) Improvements to Geometry Algorithm

whether or not a particular spectral line was rejected for use in a layer,^(a) the inclusion of Schumann-Runge band and continuum features (Minschwaner et al. 1992), and the addition of a solar spectrum model (Kurucz 1994). Changes to the program source code include vectorization of routines to increase the computational speed, parameterization of dimension statements to allow for easy changes in the size of arrays (e.g., the maximum number of layers allowed), the ability to configure the model for a variety of computers (which is aided by the parameter statements), and improvements to the atmospheric path geometry formulation. Other features of FASE include the option for output that is formatted for input to multiple-scattering programs, such as CHARTS (Moncet and Clough 1992) or DISORT (Stamnes et al. 1988), and the ability to calculate spectra over a much wider region than currently allowed by FASCODE.

Because we are combining elements of FASCODE and LBLRTM and wish to make improvements to the overall structure and use of the code, there are two key issues which must be addressed: 1) what are the origins and magnitudes of numerical differences between FASCODE and LBLRTM, and 2) what coding improvements should be adopted which would maximize algorithm speed while allowing flexibility for the user community and maintainability for the code itself. This paper addresses the second of these issues.

(a) The line rejection flag is particularly useful when computing radiance derivatives with respect to temperature using a finite-difference scheme since a line could be rejected in the reference case and not after perturbing the temperature, or vice versa. In such cases large errors would be introduced unless the line was consistently rejected.

Program Structure

An essential point to be considered in the development of FASE is the determination of the structure of the program. In the current FASE structure (inherited from FASCODE) the optical depth and radiative transfer calculations are performed at a spectral resolution appropriate for the local pressure conditions. This results in a complex algorithm for merging layers with different spectral resolution. Further, the various core modules for the calculation of molecular optical depth, aerosol attenuation, atmospheric path characteristics, filtering, etc., are grouped into a single executable code with a complex driver controlling the sequence of calls to the different subroutines to perform any one of numerous predefined functions (e.g., radiance in a clear atmosphere, radiance in a cloudy atmosphere, or weighting functions). This structure was adopted in response to a desire to reduce the number of computations and also to accommodate the needs of users not familiar with radiative transfer. Aside from the fact that an extensive set of instructional inputs must be provided by the user in order to run the code, the current structure has a serious drawback for research applications in the sense that the code cannot be easily tailored to meet specific user needs (Gordley et al. 1994) or to optimize the execution time for specific applications.

One option under study to solve this issue is to split the various core modules into independent subroutines or executable modules with clearly documented inputs and outputs. A set of simple, easily customized, standard radiative transfer routines that perform single functions would be provided, thus eliminating the need for an extensive input control file and giving the user the capability of organizing a sequence of functions to meet the requirements of a particular problem. The modules would be structured such that a novice user need only create an input file and examine the output (as with the current FASCODE), with all intermediate steps transparent to the user. However, what would be different from the current program format is that the structure of the modules would make it easy for the experienced user to rapidly implement new features or modify parameters in existing features.

As mentioned earlier, the complexity of merging layer optical depths in FASCODE/LBLRTM results from the desire to calculate layer transmittances at the local spectral resolution in order to save on the required number of exponentiations when computing the radiative transfer. However, for a non-homogeneous atmospheric path this approach requires that calculated transmittances be interpolated to the spectral resolution of the next layer.

Computational savings can only be derived with this approach by merging the successive layers from bottom to top (in the direction of decreasing pressure). We believe that this approach is obsolete since performing the exponentiations is only a small fraction of the total computer time on modern computers. Furthermore, for many applications such as multiple-scattering, inversions, etc., much greater gains can be obtained by merging the layers from top to bottom and bottom to top at the same time (Moncet and Clough 1992). Thus it is best not to attempt to satisfy the above merging constraint. Finally the spectral overlap needed for performing the interpolation defeats the requirements for parallel processing.

One way to solve this problem is to build the code around a core module which computes the molecular optical depth at the same spectral resolution for each layer. The actual computation occurs at the spectral resolution appropriate for the layer, but the result is then interpolated to the final spectral resolution (which corresponds to the highest resolution in the problem, usually prescribed by the geometric line-of-sight). The advantage of this technique is that the total spectral interval can be broken into sub-intervals with uniform end-points for all layers, making customization of the code easier. The size of these sub-intervals would depend on the amount of core memory available. Because of the uniform output for all layers, a complete calculation can be performed in memory for each sub-interval. Furthermore, this approach simplifies the extension to parallel processing of the sub-intervals.

The drawback of interpolating the molecular optical depths to the same resolution is that the radiative transfer must be computed at high resolution even for layers where a lower resolution would suffice for computational accuracy. The impact of this on the timing has been found to be minimal (Snell et al. 1995). In addition, the structure of the program is simplified, and it would be very easy for the user to adapt the modules to meet the needs of specific problems. For calculations consisting of multiple runs (different atmospheres, instrument functions, viewing geometry, etc.), this structure would be more efficient and easier to use because it would eliminate the need for multiple input files and would allow the processing of different operations in parallel (saving read/write time).

Conclusions

Creating the FASE from the existing routines of FASCODE and LBLRTM and restructuring the source code will increase the flexibility of the code and allow for easy customization of the algorithm to fit specific user problems.

Acknowledgments

AER support for this project was obtained from Phillips Laboratory (grant #F19628-93-C-0040), with partial funding from DOE/PNL ARM subcontract #218101-A-Q 1 to Phillips Laboratory. Jinxue Wang was supported by the U.S. National Research Council (NRC). We thank S. A. Clough and P. D. Brown for useful discussions.

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