VSTAR - A NEW HIGH-SPECTRAL-RESOLUTION ATMOSPHERIC RADIATIVE TRANSFER CODE FOR MARS AND OTHER PLANETS.

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Introduction

VSTAR (Versatile Software for Transfer of Atmospheric Radiation) is a new atmospheric radiative transfer software package developed at the Australian Centre for Astrobiology. It is designed to be sufficiently general to be applied to the atmospheres of the Earth, other solar-system planets, and extrasolar planets. VSTAR solves the radiative transfer problem in a plane-parallel atmosphere by combining a line-by-line treatment of the molecular absorption with a full multiple-scattering solution of the radiative transfer equation incorporating Rayleigh scattering and scattering from clouds and aerosols. VSTAR is highly portable and compiles under a range of Fortran compilers including the freely available g77 compiler. Development of VSTAR began in 2002 with most of the current code being completed in 2005. It is thus a modern system designed to fully exploit the high performance of modern CPUs and the large memory capacities now available.

Design Goals

VSTAR has been designed to support the interpretation and analysis of ground-based planetary observations. This includes, the program of near-IR spectroscopy of Mars and Venus being carried out at the Australian Centre for Astrobiology as well as other visible and IR studies of solar-system and extrasolar planets. In such studies it is necessary to predict the emergent radiance at the top of the atmosphere of the planet being observed. However, it is also important to be able to model the transmission of the Earth's atmosphere. Furthermore, both need to be modelled at a resolution that fully resolves the atmospheric lines. If this is not done it is not pssible to correctly predict the spectrum of a planet such as Mars observed at the ground in the region of strong absorption lines such as CO_2 which are present in both the atmosphere of Mars and of Earth. We have carried out simulations that show that attempting to remove these telluric absorptions by the techniques conventionally used by astronomers (division by a standard star spectrum) leads to errors of up to 50% for martian CO_2 lines.

Thus VSTAR is a high-spectral-resolution package using line-by-line methods for molecular absorption and solving the radiative transfer equation for a grid of what may easily be up to a million spectral points. Until recently such an approach was considered too computationally demanding to be feasible for general use. However, the fast CPUs available in modern desktop machines are capable of solving such problems in realistic times (1-2 hours for a typical problem).

Some other goals of the VSTAR development are as follows:

1. the software should be able to solve complete radiative transfer problems from basic data (such as line databases and aerosol refractive indices) in a single program (i.e. it should not require a series of intermediate steps and intermediate files).

2. it should be sufficiently general to be applied to the atmosphere of any planet.

3. it should be easy to use by non-experts in radiative transfer.

4. it should be freely distributable as source code (i.e. use no proprietary software).

5. it should be well documented (internally and externally).

Software Structure

The VSTAR software is written in Fortran 77 with a few widely available extensions (all part of the Fortran 90/95 standards). Fortran 77 was chosen to enable the software to be easily compiled on a range of different systems. In particular it compiles under the freely available GNU g77 compiler as well as all other Fortran compilers it has been tested with (including Intel, IBM XL and Sun). Fortran also enables the use of much existing radiative transfer and numerical software.

VSTAR is structured in a modular way and organised into a set of largely independent packages as follows:

The MOD package — This implements the concept of a "model". A model in VSTAR is defined by a 2 dimensional grid where 1 dimension specifies the atmospheric layers and their pressure, temperature and composition, and the second dimension is the grid of spectral points for which the radiative transfer calculation will be carried out. Once a model has been defined the 2D grid needs to be filled in with values for the vertical optical depth, single scattering albedo and phase function at each point. The information for this is provided by the LIN, RAY and PART packages.

The LIN package — This is used to add molecular line absorption data to the model starting from a line database such as HITRAN. It can read line data in 160 character format of HITRAN 2004 (Rothman et al. 2005) or the 100 character format of HITRAN 2000 (Rothman et al. 2003) or earlier. Line profiles are calculated using an approximated Voigt profile (Humlicek 1982, Schreir 1992) in the core and a Van Vleck-Weisskopf profile in the wings. The profiles of strong lines are calculated out to large distances from the core.

The RAY package — This package is used to add Rayleigh scattering to the model. Scattering cross sections are calculated from the refractive index of the atmosphere (Liou 2002). Two models are implemented, one apropriate to scattering in air, and one for a general mixture of gases.

The PART package — This package is used to add particle scattering (e.g. aerosols and clouds) to the model. Up to 20 different particle scatterers, each with its own height distribution in the atmosphere, can be included in a model. Precalculated scattering data can be input or scattering properties can be calculated from refractive indices and size distribution using the speherical particle Mie scattering code of Mischenko.

The RT package — This combines the results from all the other packages and performs the radiative transfer solution. It combines the molecular absorption, Rayleigh scattering and particle scattering data to give the total vertical optical depth, single scattering albedo and phase function for each layer of the atmosphere at each wavelength point. This information is then fed to the radiative transfer solver, together with boundary condition data such as direct beam sources and surface reflection properties. VSTAR is structured so that a number of different radiative transfer solvers can be incorporated, but currently is normally used with the DISORT discrete ordinate solver (Stanmes et al. 1988).

VSTAR is structured as a Fortran subroutine library, and is currently used by writing relatively simple Fortran programs to set up models. A typical program would operate as follows:

1. Create a model by specifying the atmospheric structure and wavelength grid using the MOD package. The package returns a model identifier that is used to refer to the model subsequently.
2. Add components to the model. Components can include molecular line absorbers (LIN package), Rayleigh scattering (RAY package), aerosols and clouds (PART package), direct beam sources, and surface reflection properties (RT package).
3. Perform the radiative transfer solution (RT package).

A user interface to enable models to be set up without the necessity to do any programming is a possible future addition.

Optimizations

The current version of VSTAR has been designed to ensure accurate results rather than optimized for speed. Thus line profiles are calculated in full at every wavelength point, and a full radiative transfer solution is done for each wavelength point. Despite this it can run useful models of the Mars and Earth atmospheres over substantial wavelength ranges in 1 to 2 hours on CPUs such as a 3GHz Pentium 4 or 2.5GHz G5. However, there are many applications where it would be useful to be able to run models more quickly. One optimization would be used to use an unevenly spaced wavenumber grid with closely spaced points near the cores of spectral lines and more widely separated points away in line wings. In applications where full spectral resolution is not needed, a correlated-K approach could be used to cut down the number of radiative transfer solutions. Another way of speeding up the code would be exploit multiple processor machines either in shared-memory configurations or in the form of clusters.

Examples

An example of how VSTAR can be used in intepreting ground-based observations of Mars is shown in figure 1. This simulates the observation of methane (CH_4) in the martian atmosphere using observations in the 3000cm ^{1} region (3.3 m). There have been several reports of the detection of martian CH_4 (Formisano et al. 2004, Krasnopolsky et al. 2004, Mumma et al. 2004, 2005). Methane is of great interest because of its possible biological origin. Observations of methane from ground-based telescopes are, however, complicated by the presence of strong broad telluric absorption from methane in the Earth's atmosphere. Such observations therefore, have to be made when the radial velocity of Mars relative to Earth is at a maximum.

The simulation in figure 1 involves two VSTAR models. Firstly a model for the Mars atmosphere has been used to predict the radiance at the top of the atmosphere for three cases, no methane, 10ppb methane and 50ppb methane. These spectra show a group of narrow lines of methane, as well as a number of lines of H_2O. At this wavelength most of the light is reflected sunlight, passing twice through the atmosphere. The second model is for the Earth's atmosphere, and models the Mauna Kea observatory site at an altitude of about 4200m. The transmission spectrum of the atmosphere is plotted in the

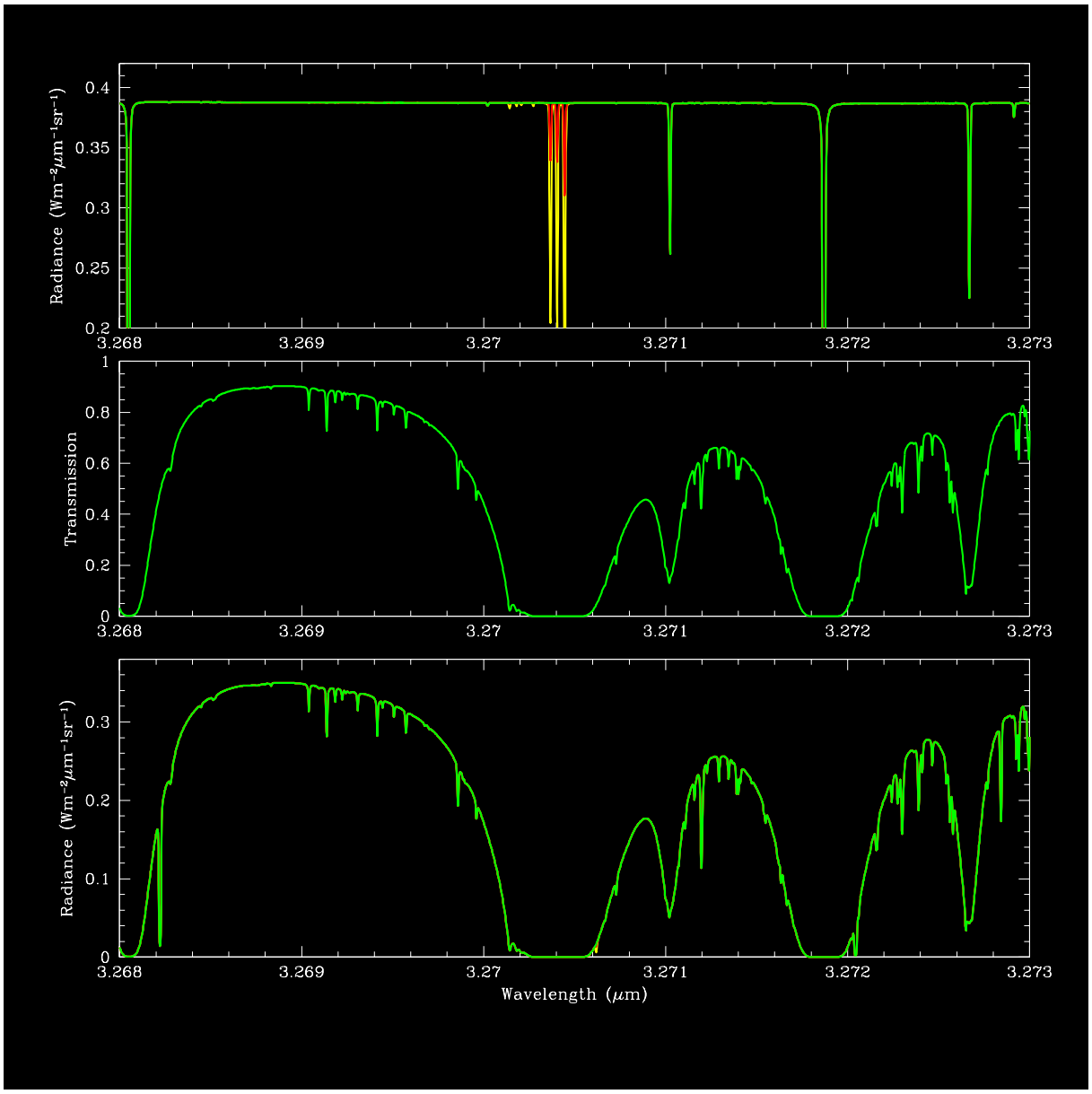

Figure 1: Examples of VSTAR model results. Top panel - radiance emitted at the top of the martian atmosphere for Mars atmosphere models with no methane (green), 10ppb of methane (red) and 50ppb of methane (yellow). Middle panel - Transmission of the earth atmosphere for the Mauna Kea site. Lower panel - Radiance as seen from the ground at the Mauna Kea site with Mars at a recession velocity of 16kms ^{1} with the same colour code as the top panel. The Martian methane lines are just visible on the edge of the broad telluric absorption at about 3.2706 m.

middle panel of figure 1. This spectrum shows the same methane and H_2O lines as the Mars spectrum but the lines are much stronger and broader owing to the higher column densities and increased pressure broadening.

The lower panel shows the result of doppler shifting the Mars spectrum for a recession velocity of 16kms ^{1} (close to the maximum value) and multiplying by the earth atmsophere transmission to give the spectrum that would actually be observed by a telescope at Mauna Kea. It can be seen that this velocity is only just sufficient to shift the methane lines into an observable wavelength. The difficulty of making such observations with a ground-based telescope is clear.

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