kCARTA: An Atmospheric Radiative Transfer Algorithm using Compressed Lookup Tables

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ABSTRACT

kCARTA is a radiative transfer code for a non-scattering Earth's atmosphere. As packaged, it can be used to output monochromatic gas optical depths, and clear sky radiances and jacobians. This Matlab package is a simpler version of the f77 version, which includes scattering and fluxes.

The code is driver by profiles in the .rtp format allowing the user to easily change atmospheric conditions as needed. US Standard Atmosphere optical depths have been precomputed and saved to a lookup table. This means (linear) interpolations required to compute the optical depths for arbitrary atmospheric profiles can be done very rapidly, as can the derivatives needed for the Jacobians. This makes kCARTA very fast.

The code in the basic Test package allows the user to do RT calculations for a downlooking instruments at the top of atmosphere (TOA), as well as code to only compute optical depths. This basic package assumes the "klayers" levels are the same as those in the kCompressed Database. NLTE radiance effects in the 4 um CO2 band are included in daytime RT calculations.

A more versatile package allows one to to use pressure layerings different than that of the kCompressed Database. This is required for uplooking instruments as the rapid variation of temperature and profile gas constituents near the instrument, require a finer layering than that of the standard kCompressed pressure layering.

We hope that the ease of use, range of features and speed of kCARTA, make it a useful tool. In addition to the main kCARTA source code, some packages need to be picked up. One is kLAYERS, which allows an user to input a radiosonde or model point profile, and output a layer averaged profile that kCARTA can use. Another is the *RTP* package, which is a AIRS Level II file format.

This document is very much a work in progress. Some major omissions include references, significant examples of kCARTA output, and comparisons of kCARTA output to observed spectra. These omissions will be rectified in the future. Please give us your feedback on both the code and the documentation!

1 Introduction

kCARTA stands for "kCompressed Atmospheric Radiative Transfer Algorithm." This is an infrared, "monochromatic" radiative transfer algorithm written for a one dimensional non-scattering Earth atmosphere.

At the heart of the code are routines to uncompress an optical depth database, computed for the US Standard Profile and for 10 temperature offsets (-50 K, -40K, ..., +40 K, +50 K) from this profile. This makes computing optical depths for any realistic Earth atmosphere very fast and accurate, as the code only needs to interpolate the arbitrary profile using this underlying temperature grid. Uncompressing the database also rapidly yields analytic temperature jacobians.

The code was originally written in F77, and morphed to include upwelling and downwelling clear sky radiative transfer calculations, calculations in a scattering atmosphere, NLTE effects in the 4 um CO2 band, and fluxes and heating rates calculations. This Matlab package encapsulates the uncompression routines, and provides examples of how to produce clear sky optical depths and radiative transfer calculations. The package is tied in with UMBC kLAYERS and "RTP" packages. The former takes a levels profile, and produces a layers averaged profile. The latter is a .hdf based file format, and allows us to include all necessary parameters (such as profile information, satellite and solar angles, emissivities) into a "Radiative Transfer Protocol" file.

2 Radiative transfer

For a downward looking instrument, in a clear sky, the surface term and layer emission terms are automatically included in the radiative transfer calculation. In addition, reflected thermal and solar terms can also be included :

$$R(\nu) = R_{surface}(\nu) + R_{layer\ emission}(\nu) + R_{thermal}(\nu) + R_{solar}(\nu) \qquad (1)$$

where the terms are the surface, layer emissions, reflected thermal and solar respectively. The reflected thermal term is computed accurately by determining (monochromatically) the layer to ground cumulative sum of absorption coefficients, and then using an optimum diffusive angle based on a parameterization of angle as a function of this cumulative sum. This makes the inclusion of reflected thermal in the code quick and accurate. By differentiating the radiance equation with respect to a layer gas amount or temperature, the radiance Jacobian is

obtained. Dropping the surface and reflected thermal terms enables kCARTA to compute the radiance measured by an upward looking instrument as well. The radiative transfer routines include effects of curvature on angles that deviate from nadir.

More documentation on the driver files, and on the convolution routines, can be found in the appropriately named pdf files.

3 Analytic Jacobians

Taking into account the view angle correction, if τ_i is the optical depth due to gas G at layer i, given by $\tau_i = q_i K_i/\mu i$ where the symbols respectively stand for optical depth (dimensionless), gas amount (kmoles/cm2), gas absorption (cm2/kmol) and $cos(viewangle)$, then the finite difference column gas jacobian is given by the difference between the new and unperturbed radiances $\delta r = r_{new} - r - 0$ when the gas amounts in layers 1 to N are perturbed by a fraction δ. The (finite differences) column jacobians can be obtained from the (gas) layer analytic jacobians using

$$\delta r = \frac{\partial r}{\partial q_1}\delta q_1 + \frac{\partial r}{\partial q_2}\delta q_2 + ... + \frac{\partial r}{\partial q_N}\delta q_N$$

or

$$\delta r = J_1\delta q_1 + J_2\delta q_2 + ...J_N\delta q_N$$

Usually we take a constant perturbation to the column ie $q_l \rightarrow q_1(1+f)$ where $f \ll 1$. Then $\delta q_l \rightarrow f q_l$ and $\delta r = f\{J_1 q_1 + J_2 q_2 + ... + J_N q_N\}$. For example, for a 2 layer atmosphere the upwelling radiance (without background thermal or solar terms)jacobian terms J_l is

$$\begin{aligned} r = \quad & \epsilon B(T_s) exp(-q_1 K_1/\mu_1) exp(-q_2 K_2/\mu_2) + \\ & B(1)(1 - exp(-q_1 K_1/\mu_1)) exp(-q_2 K_2/\mu_2) + \\ & B(2)(1 - exp(-q_2 K_2/\mu_2)) \end{aligned}$$

from which the layer jacobian terms J_i reduce to

$$\begin{aligned} J_1 = \frac{\partial r}{\partial q_1} = \quad & -\tfrac{K_1}{\mu_1}\epsilon B(T_s) exp(-q_1 K_1/\mu_1) exp(-q_2 K_2/\mu_2) + \\ & -\tfrac{K_1}{\mu_1} B(1)(exp(-q_1 K_1/\mu 1) exp(-q_2 K_2/\mu 2) \end{aligned}$$

$$J_2 = \frac{\partial r}{\partial q_2} = -\frac{K_2}{\mu_2}\epsilon B(T_s)exp(-q_1K_1/\mu_1)exp(-q_2K_2/\mu_2) + \\ -\frac{K_2}{\mu_2}B(1)exp(-q_1K_1/\mu 1)exp(-q_2K_2/\mu 2) + \\ -\frac{K_2}{\mu_2}B(2)exp(-q_2K_2/\mu 2)$$

4 kCompressed Database

Optical depths are computed for all molecules in the HITRAN database, using a profile derived from the 1962 US Standard Atmosphere. These optical depths are pre-computed using a Matlab based line by line code.

The current database spans 605 cm^{-1} to 2805 cm^{-1}, broken up into chunks that are 25 cm^{-1} wide. The point spacing of the current database is 0.0025 cm^{-1}, which is an average over five points spaced at 0.0005 cm^{-1}. One hundred pressure layers are used to generate the database, from 1100 mb down to 0.005 mb. These pressure layers are the same as those used for the AIRS (Atmospheric InfraRed Sounder) Fast Forward Model, for which kCARTA is the "Reference Forward Model."The thickness of the layers is roughly 250 m close to the surface, gradually increasing to as much as 2000m in the upper atmosphere. The 100 layers were carefully chosen so as to keep errors at the 0.1 K level, comparable to noise levels in contemporary sounders.

The temperatures in the spectroscopic database are computed at the Standard Profile, as well as ten temperature offsets (in increments of $\pm$ 10K) on either side of the Standard Profile. These optical depth tables are compressed using a Singular Value Decomposition (SVD) technique, to produce our kCompressed database.

The current spectroscopic compressed tables use the HITRAN98 database for both line-parameters and cross-sections. The full and first-order CO_2 linemixing is from refining the modeling undertaken by David Tobin. It should be more accurate than that currently in GENLN2. in addition, we have used the latest O2 and N2 continuum models (see Lafferty and J.-M. Hartmann et al in Applied Optics 1996, 1997). Other updates to spectroscopy include the "local" water lineshape as defined by CKD.

To compute the absorption coefficients for an arbitrary profile, the look-up tables are interpolated in temperature, and scaled in gas absorber amount. These interpolations allow easy computation of analytic temperature derivatives, from which we can compute temperature Jacobians. kCARTA is not limited to these 100 AIRS pressure levels/layers. The user can change the pressure levels scheme

in kLAYERS, and kCARTA will then also do a pressure interpolation (as long as the new pressures span 1100 to 0.005 mb).

The speed and features of the code make it an appealing alternative to other existing "line by line" codes such as GENLN2 and LBLRTM. The accuracy of the database has been extensively compared to GENLN2. kCARTA should contain the latest spectroscopy/lineshape information. The transmittances computed by kCARTA are smooth and well behaved, which will allow people to develop fast-forward models.

5 GasIDs

The gasIDs used by kCARTA and kLAYERS follow the HITRAN convention. "gasids_H2008" (and the earlier "gasids_H92_H2k") in this *DOC* subdirectory, provide a list of gasID vs commonly used name and/or chemical formula.

6 Units and Definitions

Frequencies are in units of wavenumbers (cm^{-1}), temperatures are in Kelvins. The gas profiles expected by kCARTA use path averages over the layers, and are in units of $molecules\mathrm{cm}^{-2}$. Temperatures should be specified in *kelvin*, while pressures and partial pressures should be expressed in *millibar*.

Output gas and mixed path optical depths are dimensionless (absorption coefficient $\times$ gas amount); obviously so are transmittances. Output radiances are in blackbody radiance units ($milliwatts\ m^{-2}sr^{-1}/\mathrm{cm}^{-1}$). Jacobians can be output in one of three modes : (a) $d(rad)/ds_m$, where s_m is the temperature or gas amount in layer m, (b) $d(rad)/ds_m \times Z_m$, where s_m is the temperature or gas amount in layer m, and Z_m is an unit perturbation (+1 K if temperature, or +gas amount in mth layer) and (c) $d(BT)/ds_m \times Z_m$, where s_m is the temperature or gas amount in layer m, and Z_m is an unit perturbation (+1 K if temperature, or +gas amount in mth layer)

7 Installing and running kCARTA

This is for the user that wants to install and use kCARTA as quickly as possible. We purposely keep this user manual short, and ask the user to examine the

"user_set*.m" codes in the Test subdirectory in great detail, so as to understand how to use the package.

7.1 Distributing kCARTA

The distribution is divided into three parts :

- Main tarfile $kcmix_matlabVYYY.tar$ where YYY is the version number. This will contain the entire source code distribution, many needed data files, and the documentation.

- kCompressed Database : about 600Mb, supplied on CDs. We supply two versions, the big endian or the little endian versions

7.2 Installing kCARTA

Having obtained the above three, the user can now proceed to install kCARTA: Untar $kcmix_matlabVYYY.tar$: this will create a main subdirectory, named PACKAGE_UPnDOWNLOOK_2011, as well as many subdirectories containing the source code, data files and so on.

```
drwxr-xr-x 2 sergio pi_strow    7 Mar 24 17:31 Test
drwxr-xr-x 2 sergio pi_strow    4 Mar 24 17:29 RTPFILES
drwxr-xr-x 2 sergio pi_strow   13 Mar 24 17:23 DOC
drwxr-xr-x 2 sergio pi_strow   12 Mar 24 15:24 CONVOLUTION
drwxr-xr-x 6 sergio pi_strow   26 Mar 24 04:49 VariablePressure
drwxr-xr-x 6 sergio pi_strow    9 Mar 23 12:40 private
drwxr-xr-x 3 sergio pi_strow    4 Mar 23 10:35 JACDOWN
drwxr-xr-x 6 sergio pi_strow    6 Mar 22 15:38 DATA
```

8 Files in directories

8.1 Main directory Usual 100 AIRS layers

This contains the main files a user should need for a pressure layering that is the same as the AIRS 100 layers.

Routines for uncompressing the database ($kcmix*.m$) and the continuum files ($cont*.m$), for doing radiative transfer ($rtchunk\_Tsurf*.m$) are included here. The $\_nojac$ extension to the name means the faster (non jacobian version), while $\_jac$ is the slower, jacobian version. The main routines are $matlab\_kcarta\_downlook_*.m$

Note : if the user wants to edit which gases he/she should be included in the "atmosphere", then look for the line that says "edit this list to only keep gases you DO want" in matlab_kcarta_downlook_jac.m or matlab_kcarta_downlook_nojac.m or matlab_kcarta_opticaldepths.m; default is to add ALL gases.

```
auxiliary_set.m
contcalc2.m
contcalc2_S_F.m
continuum_temp_interp_weights_jac.m
continuum_temp_interp_weights.m
contjaccalc2.m
dirname.m
doload.m
find_chunks.m
initialize_extra.m
initialize_kcmix.m
kcmix2jac.m
kcmix2.m
matlab_kcarta_downlook_jac.m
matlab_kcarta_downlook_nojac.m
matlab_kcarta_opticaldepths.m
nlte.m
op_rtp_to_lbl2.m
rtchunk_Tsurf_jac.m
rtchunk_Tsurf.m
temp_interp_weights_jac.m
temp_interp_weights.m
```

As given out, the code was optimized for the 605 - 2830 cm^{-1} spectral range which is the range covered by AIRS, IASA, CRiS, and HIRS and AERI instruments. However the code is flexible enough to allow optical depth and radiance calculations in other spectral bands. Since the FWHM of lines gets smaller (larger) as the wavenumbers get smaller (larger), the resolution of the database must change. Each file in each spectral range will contain 10000 points; so for example at the

default 0.0025 cm^{-1} resolution of the main IR default band (605-2830 cm^{-1}), the files each span 25 cm^{-1}. We envisage the following :

```
kcartachunks = 00080 : 0002.5 : 00150;  prefix = '/j';
kcartachunks = 00140 : 0005.0 : 00310;  prefix = '/k';
kcartachunks = 00300 : 0010.0 : 00510;  prefix = '/p';
kcartachunks = 00500 : 0015.0 : 00605;  prefix = '/q';
kcartachunks = 00605 : 0025.0 : 02830;  prefix = '/r'; ** default **
kcartachunks = 02830 : 0025.0 : 03580;  prefix = '/s';
kcartachunks = 03550 : 0100.0 : 05650;  prefix = '/m';
kcartachunks = 05550 : 0150.0 : 08350;  prefix = '/n';
kcartachunks = 08250 : 0250.0 : 12250;  prefix = '/o';
kcartachunks = 12000 : 0500.0 : 25000;  prefix = '/v';
kcartachunks = 25000 : 1000.0 : 44000;  prefix = '/u';
```

It is the responsibiliy of the user to set fA,fB in the "user_set_input*" files such that they only span *ONE* spectral range. For example, one run covering 605-2830 cm^{-1} is fine, as is another run covering 500-605 cm^{-1}. But the code as written will not permit a single run covering 500-2830 cm^{-1}.

8.2 private

This subdir contains files that are called by the main routines, and should not be modified.

8.3 DOC

The documentation for this package

8.4 CONVOLUTION

Convolution routines. We include generic gaussian convolvers, as well as AIRS SRF convolvers, and IASI/CRiS convolvers. Note the files contained in this subdir will not be supported.

8.5 JACDOWN

This has the main driver for a downlook jacobian calculation, "jac_downlook.m" which calls files in the *private* subdirectory underneath this. One can speed up the jacobian code by eg removing the looping over the weighting functions, or over the temperatures.

8.6 RTPFILES

Sample rtpfiles for this package; "desert" is a downlooking case at 100 AIRS layers, while the other is an uplooking case at a different layering scheme. In addition we provide a subdirectory with some binary files output from the f77 code.

8.7 DATA

Contains subdirectories with continuum, solar, NLTE and CO2 Chifunction datafiles.

8.8 Test

Examples of two driverfiles, one which computes optical depths (based on a list the user supplies), and the other which computes radiances (and jacobians if asked). The user should carefully examine these files, as they provide a working outline of how to use this package.

Basically, the user is allowed to set the following parameters : which HITRAN version to use, start/stop wavenumbers for the calculations, whether or not to do Jacobians, what output units for the Jacobians, what CKD version, and name of input rtp file.

```
user_set_input_downlook.m        parameters driving dokcarta_downlook.m
user_set_input_opticaldepths.m   parameters driving dokcarta_opticaldepths.m
```

The user needs to supply paths to where the solar files, continuum files, nlte files, klayers executables, optical depth database and reference profiles are; this is controlled via *user_set_dirs.m*

```
user_set_dirs.m                  set up the paths to directories
```

Finally the user can commence the computation, calling one or the other of the routines named below (which call relevant files from above).

```
dokcarta_downlook.m              compute RT
dokcarta_opticaldepths.m         compute optical depths
```

This subdir also includes two matlab files, containing radiances output using H2004 and H2008.

8.9 VariablePressure Different pressure layers

This contains the main files a user should need for a pressure layering different than the AIRS 100 layers. This makes the code(s) slower. The structure and content of the directories is the same as before *viz*

```
drwxr-xr-x 2 sergio pi_strow    10 Mar 24 04:49 Test
drwxr-xr-x 6 sergio pi_strow     8 Mar 23 11:58 private
drwxr-xr-x 3 sergio pi_strow     4 Mar 23 10:36 JACUP_VarPress
drwxr-xr-x 3 sergio pi_strow     4 Mar 23 10:35 JACDOWN_VarPress
```

Test has dokcarta_downlook.m, dokcarta_uplook.m (very similar to the "downlook" case) and dokcarta_opticaldepths.m.

JADOWN_VarPress has jacobian routines for downlooking instruments

JACUP_VarPress has jacobian routines for uplooking instruments

9 Comparisons against f77 and our code

We have tested this code against the f77 kCARTA code and across the IR bands, have errors less than 0.05 K in brightness temperature. The speeds are also very similar (roughly about 60 seconds on a 2.6 GHz processor for a full radiative transfer calculation).

The *Test* directory contains "matlab_test_desert_0725_2004.mat" which is a radiance computation coming from running the "dokcarta_downlook.m" in that directory.

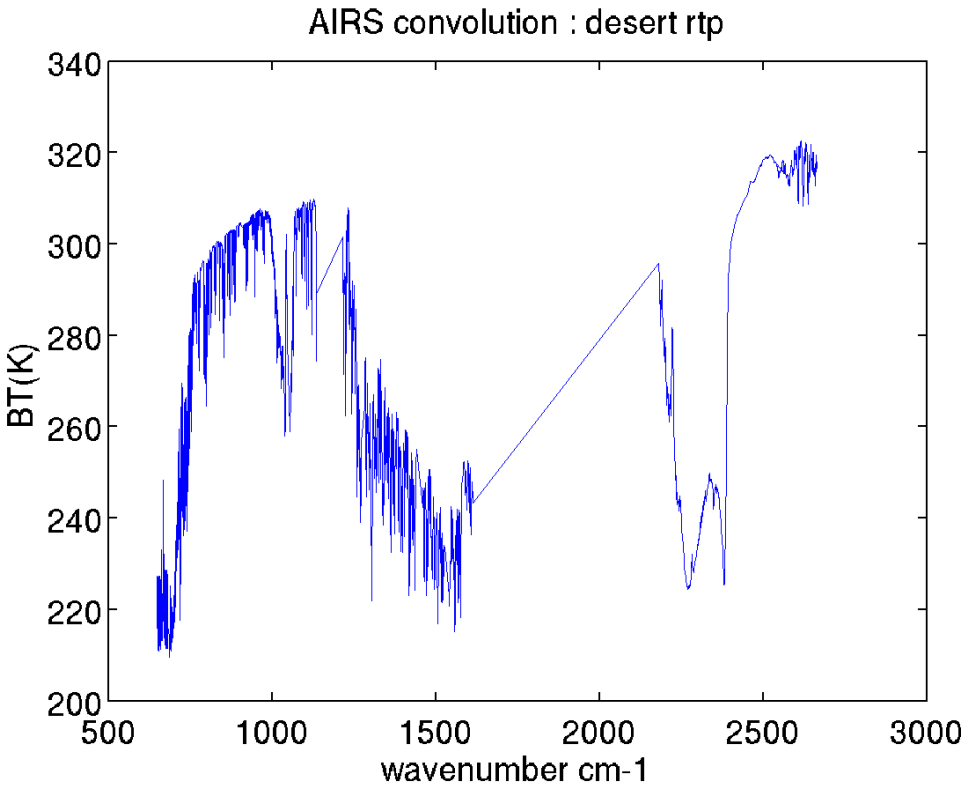

Figure 1: Sample output from "desert_op.rtp", convolved with AIRS SRFs