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Interactive comment on "kCARTA: A fast pseudo line-by-line radiative transfer algorithmwith analytic Jacobians, fluxes, Non-Local ThermodynamicEquilibrium and scattering for the infrared" *by* Sergio DeSouza-Machado et al.

Anonymous Referee #1

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kCARTA: A fast pseudo line-by-line radiative transfer algorithm with analytic Jacobians, fluxes, Non-Local Thermodynamic Equilibrium and scattering for the infrared

by S. DeSouza-Machado et al. August 2019.

Referee comments.

OVERVIEW

The paper describes an 'intermediate' radiative transfer model kCARTA: faster than the line-by-line model (eg UMBC-LBL) but slower than the models used in operational pro-

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Discussion paper

cessing of data from the new generation of hyperspectral instruments (eg SARTA). As a monochromatic model, this has the advantage of using Beer's Law to combine transmittances but relies on pre-computed absorption coefficients at a fixed set of pressure, temperature and (for H2O) mixing ratio points, which introduces a (small) interpolation error compared with line-by-line models.

With increasing spectral resolution of instruments and increased computing power, monochromatic models such as kCARTA may soon form the basis of operational retrieval or assimilation schemes (eg the OSS model), so this represents an important development and the algorithms should be documented in a journal such as AMT. However, there are several major issues with the current paper that I feel should be addressed.

GENERAL COMMENTS

1) There is no comparison of kCARTA radiances with a more well-established (and preferably line-by-line) model, not even the source models UMBC-LBL or LBLRTM. The kCompressed tables have been previously verified to reproduce the absoption coefficients or optical paths, but this paper deals with all the extra components of a radiative transfer model.

2) I have concerns about the impact of the coarse spectral resolution: 0.0025cm-1. Where does this figure come from? The usual requirement for radiative transfer is to be able to capture the signal from Doppler-broadened lines in the upper stratosphere, which have typical mid infrared widths of 0.001 cm-1, hence resolutions of 0.0005 or 0.001 cm-1 are generally considered necessary. Given the inherent flexibility of the kCompressed tables, I am also surprised that the authors have not considered using an adaptive, rather than fixed, spectral grid, so that the spectral resolution is concentrated around the line-centres, so obtaining better accuracy for the same size compressed datasets and computation time.

3) I am unclear on the conversion of atmospheric profile quantities (temperature, pres-

sure, composition) to the (presumably?) equivalent homogeneous paths represented by the kCompressed data. Are these absorber-weighted equivalent (ie Curtis-Godson) temperatures and pressures? Or simply layer means? Given the use of a spherical atmosphere (what radius of curvature is assumed?) rather than a plane-parallel assumption, presumably some sort of numerical integration scheme is required to obtain these quantities, even the total amount of absorber in a layer.

4) Section 4, on the impact of spectroscopy on TOA radiances, seems an unnecessary digression. While spectroscopic uncertainties are certainly an issue that merits attention, that's not really anything to do with the kCARTA model being introduced (besides which all the variation is handled in the generation of the kCompressed datasets, which are to some extent independent). The data gap in the plots, arising from the gap in AIRS coverage, is also undesirably for such a comparison. It would have been more useful to see comparisons of kCARTA TOA radiances against other models instead.

5) For most molecules, kCARTA uses data created by the UMBC-LBL model using the Van Vleck and Huber lineshape. Since the Voigt lineshape is very much the 'standard', there should be some explanation of how this differs and why it is used in preference to Voigt.

6) The inclusion of non-LTE effects, just for the CO2 4um band, seems to require the inclusion of a separate line-by-line model within kCARTA. This is a huge overhead in complexity for a relatively specialised application. Given the kCARTA structure, it seems a more natural approach would have been to incorporate vibrational temperature as an extra axis on the kCompressed datasets, and just use GENLN2 to calculate these. Alternatively, if you are including a LBL model within kCARTA, at least extend it so that LBL (with or withouth non-LTE) can be used for any molecule.

7) The calculation of background thermal radiation (section 7) uses an interesting idea, and would probably have merited some expansion as a separate (if somewhat specialised) article by itself. I have a number of questions, detailed in the minor comments

below.

TYPOS/MINOR COMMENTS

P1 L20: '... data are presently ...'

P1 L20: Given Susskind was describing cloud clearing for the previous generation of meterological instruments I'm not sure it's an appropriate reference for the hyperspectral instruments.

P1 L20: The text may be read as implying that there is some sort of correction applied to the spectra to remove the influence of clouds, whereas I suspect it is more accurate to say that any cloud-contaminated spectra are simply rejected.

P2 L27: What determines this 0.0025cm-1 figure? As a rough estimate I expect it would be determined by the requirement to resolve the Doppler widths of lines, and given molecular velocities are of the order of c/10ˆ6 that would correspond to around 0.001 cm-1 at 1000 cm-1.

P2 L27: I am not convinced by the argument that the computation of optical depths at high spectral resolution for 50 or so profiles for the training set is something that needs accelerating. Surely this is something that only has to be done once and, even if occasionally repeated, the fact that it takes a week rather than a couple of hours isn't really be an issue.

P2 L40: I assume the issue with replacing line-by-line with kCompressed data is one of the accuracy of the absorption coefficient or reconstructed layer optical depths. However to state that the 'radiances' are accurately reproduced requires a whole new set of tests to verify the accuracy of the radiative transfer through an atmosphere.

P2 L49: Missing second ')' after 1999.

P3 L71: I have not come across the Van Vleck and Huber lineshape. Is this different to the more conventional Voigt? If so, how, and why the unconventional choice?

Fig 1: I appreciate this is just a sketch, but the black Total line doesn't seem to be a sum of the red, blue and green lines. Also raise the '-1' in the x-axis title to a superscript (and in subsequent figures).

P4 L98: Regarding MonoRTM - what is the point being made here?

P5 L107: +/- 50K does not seem a large range in temperature. Do you have any evidence that it spans the full range of atmospheric variability?

P5 L108: 'contains'

P5 L122: HITRAN 2016 lists two further isotopologues for water vapour containing a single deuterium atom and either a 17O or an 18O oxygen isotope (these are HITRAN isotopologues 5 and 6). Are these included with HDO or with the remaining H2O isotopologues?

P6 L144: It is not clear why the cross-section molecules are also represented using kCompressed databases. Presumably these end up much larger than the original files, which usually have only a few tens of (pressure,temperature) points and a much coarser spectral axis. Also using CIA probably won't work with LUTs - how will these new data be used?

P6 L150: HITRAN 2016 lists 49 rather than 42 molecules, and a number of these (or even 1:42) are not represented in the US Standard Atmosphere.

P6 L158: 'Schwarzschild'

P7 Eq(3): The solid angle integration should just be over a hemisphere and should include the B.dt/ds term scaled by cos(e) where e is the elevation angle 0:pi/2 in the hemispheric integration (thus the integral of cos(e).dOmega from 0:2pi on its own should yield pi).

P7 Eq(3): I don't see why the cos(theta_sun) appears in the last term on its own, but it seems there should be some solid angle integration over the sun's disk (as in Eq 6)

C5

otherwise it will be as if the whole sky radiates at the solar temperature.

P7 L170: Isn't 1-epsilon_s(nu) the same as rho_s(nu)?

P7 L171: extra comma near end of line

P7 L171: There is no tau_i term in Eq(3), just tau and tau_atm.

P7 L180: Assuming the temperature profile is specifed at points P,H1,H2 etc what constant temperature is assumed for, eg the lowest layer? Is it T(P), T(H1), or something else?

P7 L182: By 'density effects' do you mean refraction?

P7 L186: Both emissivity *and* reflectance have to be supplied? Eq(4) only uses emissivity.

P8 Eq(5): The indexing doesn't seem to work. Interpreting tau_(i+1 to N) as the transmittance from the base of layer i+1 to the base of layer N the calculation for layer 3 in the diagram would be (1 - tau_3).tau_(4 to N) but here N=4 so tau_(4 to N) = 1 whereas it should be the transmittance through layer 4. Similarly Eqs 8-10

P8 L195 Better to swap sections 3.3 and 3.4 to match the same order these terms appear in Eq (3)

P8 L196 rho is now defined as reflectance, but for Eq 3 it was reflectivity. Is there a difference?

P9 L213 As a general comment, it would be nice to have a plot of the magnitude of these four terms as a function of the infrared spectrum, assuming say some fixed surface emissivity of around 0.98 (so 2% diffuse reflectance).

P9 Section 4: Presumably for this exercise different sets of kCompressed databases were computed by running UMBC-LBL etc for the different sets of spectroscopic data, and then running kCARTA using these 3 different sets of kCompressed databases.

If one really wants to demonstrate the differences in TOA radiance couldn't one simply run the LBL models with the different spectroscopic data and eliminate the whole intermediate step of generating kCompressed datasets?

P9 L230 'linemixing'

P10 L243 'sagain' ?

P10 L247 it is not clear that differences have anything at all to do with linemixing - it seems they might simply reflect differences in the standard line widths that would be evident whether line-mixing effects were included or not?

P13 Section 5: It seems odd that kCARTA has a non-LTE line-by-line module - it is something I would have expected in the UMBC-LBL code. Have you considered modelling non-LTE using kCompressed datasets? That would seem more in keeping with the overall design. Perhaps you would need an extra tabulated dimension in vibrational temperature, or (vib-kin) temperature?

P13 Eq 9: Summations should be from i=1,N. Also, tau_(i+1 to N) in second summation should have (ν) afterwards.

P14 L304: 'Jacobian' from here to the end of the section start to be capitalised - inconsistent with earlier 'jacobian'

P14 L305: How is dB/dT calculated? (where $s\_m = T\_m$).

P14 L310: I don't understand the last sentence - what's the difference between the Jacobian and the weighting function wrt surface temperature and emissivity?

P14 L320: 'contributes'

P15 L334: the $d\mu$ should come after the $\exp(-x/\mu)$.

P14 L334: Is there any significance in labelling this integral as E_3 ?

P14 L334: No closing bracket to match '('.

P14 Eq 13: From discussing downward radiation, the introduction of reflectance rho_s suggests to me that you are now modelling the reflected component of this radiance just above the surface. Where does the 2pi come from? I think you need to explain some of the intermediate steps.

P14 L340: If I understand this correctly, instead of approximating the downwelling radiance as if it comes from a fixed angle cos=3/5, you are adjusting the angle for each atmospheric layer according to the surface-layer optical thickness x.

It would be nice to see some plots of the comparisons with a full hemispheric integration to show that this is sigifnicantly more accurate than the fixed angle assumption. Also, is there a reason why the cut off at 30deg has to be applied for optically thick atmospheres? Otherwise it might also be useful for modelling the radiance viewed by upward-looking instruments, or downward looking instruments close to the surface.

P15 L346: Given the rapid spectral variation in any 25cm-1 interval, I don't understand how you can assign a single assumption to the whole interval. Won't there be a whole range of optical thickness within the 25cm-1 region so that the assumption works better for some spectral points than others?

P15 Sec 7.2: The linear-in-tau model, where optical depth is scaled by the sec(theta) to allow for off-nadir viewing angles, assumes a plane plane-parallel atmosphere where theta is fixed for the layer (and the same for every layer). How is this handled for the spherical atmospheres assumed in kCARTA where cos(theta) can vary significantly when viewing off-nadir?

P16 L365: It depends what you mean by the 'average layer temperature'. For the optically thin limit you would expect this to converge to the Curtis-Godson temperature, ie the absorber-weighted mean temperature, which would generally be at an altitude below the layer mid-point.

P16 L377: Even though it largely disappears after convolution (presumably because

the AIRS spectral resolution means that the radiance is dominated by contributions from lower altitudes), this 10 K difference does seem to be a serious issue. And one which would limit the use of kCARTA for accurately representing finer resolution instruments. Is this really due to not implementing linear in tau or could it be that kCARTA only uses a crude representation of layer temperature rather the something more physically justified such as Curtis Godson temperature? Why doesn't kCARTA just use the linear-in-tau model?

P17 L390 'computes'

P17 Flux Computations: are these with spherical or plane-parallel atmospheres?

P17 L407: Given the differences found from the linear-in-tau model in the previous section, could the differences in heating rates at high altitude simply be another manifestation of the same problem, ie assumption of constant temperature within thick layers at higher altitudes?

P18 Fig 6 caption: should be '0.0005' instead of '0.005'.

P18 L425: 'accuracy of its spectroscopic database'. I assume this refers to the kCompressed tables used as kCARTA input as opposed to the usual meaning which would be HITRAN or GEISA spectroscopic databases. But comparisons against GENLN2 or LBLRTM wouldn't just be a comparison of the kCompression with the original HITRAN unless your tests were for simple homogeneous paths where transmittance could be verified independently of other model assumptions such as ray-tracing and integration through atmospheric layers.

P19 L434: '0.0025 cm-1 is good enough for nadir hyperspectral sounders' - this is a contentious statement, and needs some justification (there is none in this paper).

P21 Table B2: lists (6) Direction as downwelling by default, upwelling as an option. Isn't it the other way around?

P22 L488: extra ')'.

P22 L495: 'up to'

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