Making New Corrk Directories

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1) Obtain the kspectrum folder. It comes originally from Vincent Eymet's website, but if you want the version we've been using, ask Jérémy, Laura, or Robin Wordsworth. There is a user manual made by Vincent, it is located at https://code.google.com/p/kspectrum/. You can look at it if you are interested in more details. Once you have the kspectrum folder, look inside. You will find several folders: corrk_data, kdistribution, source_std, kspec_1, and utilities.

2) If you go inside kspec_1/data/, you will find a file called "molparam_hitran2008". This lists all of the gases for which there is data available, and what they should each be called. Their names are usually straightforward, like "H2O". You don't need to do anything here, just be aware of all of the possible gases that exist.

3) Go into kspectrum/corrk_data/. There should be a folder in there named after some mix of gases that someone else has already made. Copy or rename this directory make a new directory for your new mix of gases. Example name: CO2_SO2_H2Ovar/. This would be for a mix of CO_2, SO_2, and H_2O, where H_2O is a variable gas. Inside this folder you will find some files: Q.dat, T.dat, p.dat, make_composition_gen.exe, composition.in. There will also be folders with numbers like 19x18 or 32x36. Eventually you will erase these folders and replace them with new ones, but don't do it just yet because you can use them as templates for making your new files. You can erase composition.in, because we will make it again in a moment.

4) We begin by making a large table which includes all of our desired mixes of gases in all of the temperature and pressure regimes in which we will need them. The GCM will use this table to make its radiative calculations, interpolating for intermediate values.

5) To begin, look inside Q.dat. This file specifies the gases mixing ratios. You will see something like this:

3	# of gases that you want
CO_2	Names of gases that you want
SO2	
H_2O	The last gas on the list can be a variable gas
7	Here you specify a range of possible mixing ratios of the variable gas
1.00e-7	If there is no variable gas, it is only necessary to put the mixing ratio
1.00e-6	of the last gas listed.
1.00e-5	
1.00e-4	
1.00e-3	
1.00e-2	

```
1.00e-1
```

Ex: If there is no variable gas, it would look more like this:

```
    1
CO2
    1
1.0
```

We will define the mixing ratios of the other gases later on.

6) Look inside T.dat

```
   7
100.0
150.0
200.0
250.0
300.0
350.0
400.0
```

This specifies the range of temperatures (in K) for which you need spectra. The trade-off is between flexibility (large range of temperatures) and size (the size of your table is going to be Q x T x p). Try to imagine the extreme temperatures for your situation and add a buffer on either end.

7) p.dat is similar. You will see a number at the top, which represents the number of p levels you want, and a bunch of numbers below indicating what the actual pressures are. They are in log millibars, i.e., the one below goes from 1e-3 mbar to 100 bar (1e5 mbar):

```
    9
-3
-2
-1
 0
 1
 2
 3
 4
 5
```

8) Once this is done, run “make_composition_gen.exe”. It will ask you for the name of your atmosphere; you can put the same name as your folder. Here is where it will ask you for the volume mixing ratios for your non-variable gases. Keep in mind that these values are then normalized with respect to your variable gas: i.e., if your variable gas is 50% of the total, putting a mixing ratio of 0.9 for CO_2 and and 0.1 for SO_2 would result in an atmosphere that is 50% H_2O, 45% CO_2, and 5% SO_2.

9) This process will result in a file called “composition.in”. If you look inside you will see a huge table of values representing all of the permutations of Q, T, and p. [Aside: If you are ever curious to look at one particular spectrum, this table lists the order of the spectra… so you can find it among all of numbered spectra you will produce (k001, k002, k003, etc.)]

10) Return to the kspectrum folder. Go back into kspec_1. This is your working directory. You can make a copy of it if you want to run several gas mixes at once. Copy composition.in from your corrk/CO2…/ folder into the “kspec_1/data/” folder.

11) Open the file kspec_1/data.in. There you will find “minimum atmospheric level”. Make sure this is set to 1. Set “maximum atmospheric level” to the number specified at the top of composition.in.

[TRICK: this program creates a LOT of files, which are stored temporarily in a folder called kspect_1/optimizations. It can cause you to reach your quota fairly easily. It also runs for a really long time, and can exceed your wall clock limit. As it is running make sure to go into optimizations from time to time to delete all of these accumulating files. You can delete all but the last group of files that is currently being used. If the code crashes because you run out of time or space, check optimizations/ to see what spectrum it was creating when it crashed, and then come back into data.in and set “minimum atmospheric level” to this value. Start the code again. For this reason, in the file “options.in”, the option “Compute for (1) every level defined in composition file or (2) a limited number of levels” is set to (2) so that it doesn’t recomputed the entire table of spectra every time you restart.]

12) Submit the job. On gnome you can run it in parallel using the command “llsubmit run_kspec” run_kspec is just a wrapper for the actual program, kspectrum.exe.

13) Empty out those optimization files periodically or suffer the consequences! It will take a few days to run.

After it is done….

14) Make sure the code has deleted all of the remaining optimization files. Move everything that is in the kspec_1/results into kspectrum/corrk_data/CO$_2$…/hires_spectrum/

15) Copy from corrk_data to kspectrum/kdistribution the Q.dat, T.dat, and p.dat files that you made before.

16) From here on out everything will be calculated in serial, so if you want to move to a non-parallel machine for more space, this is your opportunity.

17) Make a link from the kdistribution folder to your hires_spectrum folder: corrk_data/CO$_2$…/hires_spectrum/.

Like this:

```
ln -sf …/kspectrum/corrk_data/CO2_SO2_H2Ovar/hires_spectrum hires_spectrum
```

18) Now you need one of the folders like 19x18 or 32x36. There might already be some in kdistribution, or you can find them in corrk_data as well. Inside these

files you will find files called “narrowband_IR.dat” and “narrowband_vis.dat”. Inside they might look like this:

```
19
 10.0    140.0
 140.0   230.0
 230.0   330.0
 330.0   440.0
 440.0   560.0
 560.0   700.0
 700.0   840.0
 840.0   1000.0
 1000.0  1160.0
 1160.0  1340.0
 1340.0  1540.0
 1540.0  1760.0
 1760.0  1910.0
 1910.0  2200.0
 2200.0  2530.0
 2530.0  2900.0
 2900.0  3320.0
 3320.0  3820.0
 3820.0  4400.0
```

The number says how many bands there are, this time it is 19 in the IR. The other numbers show the positions of the bands. This part can be delicate and technical. You want your bands to be concentrated at the peak of the Planck function, where most of your energy will be found. You also want them to extend out far enough so that you aren’t losing a lot of energy at the tail end of your Planck function. You have to cut your Planck function off somewhere, but the energy inside the chopped tail will be redistributed among the other bins when it is normalized, so it is best to chop it off at a wavelength where there is only a low amount of energy. Take a look at your spectrum and make sure that you aren’t placing a band half in a window and half in an absorption. Also make sure your band density is great enough to accurately represent your important absorptions. [You can look at your spectra by plotting any of the “results” files, the first column versus the third column.] Columns: 1. Wavenumber (cm^{-1}), 2. mean molecular cross-section of the mixture (cm^2/particle), 3. absorption coefficient (m^{-1}).

19) Open run_kmatrix. Change “BANDS_DIR“ to reflect the number of bands that you want (IR first, then VIS). Change the path on the next line to whatever your path is to this file …/kspectrum/utilities/generate_kmatrix.exe. This program will run kmatrix twice, once for the IR and once for the VIS bands.

20) Submit run_kmatrix (e.g., for gnome: llsubmit run_kmatrix).

21) Copy the folder that you have made (ex: CO2_SO2_H2Ovar/) into your datagcm/corrkdata/ folder. Now you can use it by indicating the folder in callphys.def.