GAS MIX
version 1.0.0
User Manual

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Contents

1 Description of the code

1.1 Production of high-resolution spectra and k-distribution data sets

GAS MIX is part of a chain of tools designed to compute high-resolution absorption spectra of gas mixtures. At the present time, these tools include:

- KSPECTRUM: computation of high-resolution absorption spectra for any gas mixture, in any thermodynamic conditions, with a control of the uncertainty. Input data consists in public Line-by-line databases (HITRAN, HITEMP, CDSD).

- KDISTRIBUTIONS: computation of k-distribution data sets from high-resolution absorption spectra.

While the computation of high-resolution absorption spectra is possible using KSPECTRUM, these computations require massive CPU time. Moreover, using KSPECTRUM is not easy because of the many options the user has to provide. Finally, the resulting spectra are intermediate results in most cases, where the user has to use a second tool (KDISTRIBUTIONS) in order to compute the k-distribution data set associated to each high-resolution spectrum.

The purpose of GAS MIX is to provide a (certainly neither complete, neither perfect) solution to the above issues. GAS MIX 's input is the same as KSPECTRUM input: a description of the thermodynamic conditions (pressure and temperature) and of the mixture (name of the molecular species and their respective molar fractions), along with some information about the spectral domain results are wanted for: $[\nu_{min}, \nu_{max}]$. GAS MIX will then compute high-resolution spectra, at a much higher speed than KSPECTRUM would, and the associated k-distribution data sets when required, in a single step. In addition, the user does not have to provide as much information as KSPECTRUM requires (whether of not sub-lorentzian profiles have to be used, what accuracy levels have to be reached, what kind of spectral discretization scheme has to be used, etc).

Of course, autonomous behavior and faster computations means some compromises have been made...

1.2   How it works

The main idea behind GAS MIX is that the code will not actually compute high-resolution absorption spectra. It will only interpolate known reference spectra. It means, of course, that reference high-resolution spectra have to be available. They must be computed using KSPECTRUM. Therefore, KSPECTRUM is still needed, but once reference results are available, GAS MIX will be able to use them in order to perform faster computations. The main consequences are:

- The user should be aware of what KSPECTRUM did when computing reference spectra: whether or not sub-lorentzian profiles were used, whether or not line profiles have been truncated, what isotopes have been taken into account, their respective abundances, etc.

- GAS MIX will interpolate spectra in the space of reference spectra. It means that the more reference spectra are available, the more accurate results will be. Moreover, reference spectra can be added to the collection of available reference spectra at any time, thus increasing the accuracy of GAS MIX results.

GAS MIX needs the description of at least one gas mixture: let be P and T the pressure and temperature of the gas mixture, composed of n molecular species of respective molar fractions x_i.

For any species index i, reference spectra have to be available for:

- $N_{P,ref}$ values of pressure.

- $N_{T,ref}$ values of temperature.

- $N_{x,ref}$ values of concentration.

Values of $N_{P,ref}$, $N_{T,ref}$ and $N_{x,ref}$ can be different for each species.

For any species index i, $N_{P,ref} * N_{T,ref} * N_{x,ref}$ reference spectra are therefore available. GAS MIX will then interpolate $k_{a,\nu}$ for the required P, T, x_i conditions, along the required $[\nu_{min}, \nu_{max}]$ spectral interval (of course, reference spectra have to be available over this spectral interval). GAS MIX is autonomous, which means that it can use various interpolation schemes in the (P, T, x) space: linear interpolation when little data is available, cubic spline

interpolation when possible. The code will identify by itself the files that contain reference spectra that have been computed using KSPECTRUM. When no reference spectra is available for a given species, an error occurs.

For any wavenumber ν, GAS MIX will interpolate the absorption coefficient $k_{a,\nu}^{interp}(P,T,x_i)$ for the (P,T) conditions, for each species i, at the required concentration x_i. The final step is to sum every contribution in order to compute the absorption coefficient of the gas mixture:

$$k_{a,\nu}^{interp}(P,T,mixture) = \sum_{i=1}^{N} k_{a,\nu}^{interp}(P,T,x_i) \tag{1}$$

2 Installation and prerequisites

2.1 First thing to do

is to declare your fortran 77 compiler in the F77 environment variable. In order to do so, you should export this environment variable in your .bashrc, .cshrc or .profile file; for instance, add the following line into your .bashrc file:

>export F77="g77"

in case you are using the GNU fortran 77 compiler (g77). Replace "g77" by your local fortran 77 compiler if needed (gfortran, ifort, pgf...)

Then you need to type:

>source .bashr

in order to take the modifications into account. Replace ".bashrc" by whatever you are using. The purpose of defining the F77 environment variable is to provide the correct compiler to compilation commands that will be used later. If this variable is not defined, the name of your fortran 77 compiler will be asked every time a compilation will occur.

Then you need to use script "install_gas_mix.bash" that is provided with the archive. This script should be placed in the same directory than the provided zipped archive. Use command "./install_gas_mix.bash" in order to run it. This script will:

- Untar the archive, if the corresponding version of GAS MIX is not already installed

- Go into the "data" directory, compile program "make_data.exe" and run it in order to generate test files "composition.in" and "narrow-bands.in" (see section 3.2).

- Erase the zipped archive, and erase itself.

Then you can go into the newly created directory (named "gas_mixX.X.X" with "X.X.X" the version number) to continue the installation.

2.2 Tweaking the "Makefile"

Before compiling, you will have to find out what compilation options are right for your compiler, and your machine. Open the "Makefile" file, and

look at variables "FOR", "ARCH" and "OPTI". Variable "FOR" is used to specify your fortran 77 compiler.

Variable "ARCH" is used to specify machine architecture. "-m486" is probably a good choice for a PC running a 32bits linux. Use the documentation of your fortran compiler to find out what architecture option you can use.

Variable "OPTI" is used to specify code optimization options. The default options should be enough.

You might also want to set variable "DEBUG" (look for its definition in the file). You can expect faster execution times if you leave it empty.

2.3   Setting up array sizes

One limitation of fortran 77 code is that you must define array sizes before compilation. Arrays sizes used by the present code are defined within the "includes/max.inc" file. You should at least look at it before compiling, and more precisely at the value of variable "Nk_mx". Its default value is 50000 (5.10^4). You can enable a lower value if you do not have enough memory, or a higher value (which means faster execution times) when possible.

2.4   Compilation

Once you checked compilation options and array size definitions, you can use the following command in order to compile the executable file:

> make all

If compilation fails, use the compiler error message to determine what went wrong. The most probable error causes are: a bad definition of architecture compilation option, or an inappropriate value in code optimization options.

If you ever need to modify the source files (in directory "source"), you can quickly recompile the code using "make all" again. This will only recompile the modified source files, and link objects files in order to produce the new executable file.

If you have to modify the value of any variable defined in includes files (directory "includes"), you will have to recompile the whole code from scratch. Use the following command to erase all objects files, and then recompile them properly:

> make clean all

Odd errors may happen if you change an include file and then recompile using only the "make all" command (old value of the modified variable will remain in the unchanged object files).

2.5   Definition of the reference spectra folder

GAS MIX will need to know where the reference high-resolution spectra files are located. The user has to define a symbolic link named "hires_spectrum" within the "data" folder to the main folder that contains reference spectra files. These files can be organized in sub-folders, as long as they have been produced by "KSPECTRUM". For instance, let us say your reference spectra files are contained in the folder:

$HOME/Username/Spectral_data

Within the "Spectral_data" folder, you can for instance organize reference spectra files by molecule name. Therefore, you will have a number of sub-folders within your main "Spectral_data" folder:

$HOME/Username/Spectral_data/H2O

$HOME/Username/Spectral_data/CO2

$HOME/Username/Spectral_data/NO

$HOME/Username/Spectral_data/O3

etc...

Then within each one of these sub-folders, you will have a number of sub-sub folders, one per concentration level:

$HOME/Username/Spectral_data/H2O/m1 is for $x_{H_20} = 0.1$

$HOME/Username/Spectral_data/H2O/m2 is for $x_{H_20} = 0.2$

etc...

$HOME/Username/Spectral_data/CO2/m1 is for $x_{CO_2} = 0.1$

$HOME/Username/Spectral_data/CO2/m2 is for $x_{CO_2} = 0.2$

etc...

each one of these sub-sub folders contain a number of reference spectra files, one for each (P,T) level.

But you can choose any other organization, as long as every reference file is located within the "Spectral_data" folder. You need to link this folder using a "data/hires_spectrum" symbolic link, i.e. you need to type the following commands:

> cd data

> ln -s $HOME/Username/Spectral_data ./hires_spectrum

GAS MIX will navigate within the folder hierarchy of the main data folder ($HOME/Username/Spectral_data in this case) and will identify each file that has been produced by KSPECTRUM, along with the thermodynamic conditions it has been produced for. The user should only be sure that:

- Reference spectra are available for each one of the molecular species that will be required by GAS MIX .

- Reference spectra are avaiblable along the spectral intervals that will be required by GAS MIX .

3 Using the code

3.1 User input files

There are two files in the main GAS MIX folder: "data.in" and "options.in". The "options.in" file is where the user can chose between several options. The "data.in" file is where the user can specify the numerical values of a number of variables the code will use. Below is a description of these two files.

3.1.1 The "data.in" file

- First and last levels to use: the code can run for a limited number of pressure and temperature levels (see "options.in"). When using a limited number of levels, the indexes of the first and last level to use must be indicated in this file.

- First and last narrowband intervals to use: the code can run for a limited number of spectral narrowband intervals (see "options.in"). When using a limited number of intervals, the indexes of the first and last intervals to use must be indicated in this file.

3.1.2 The "options.in" file

- Section "Production of interpolated spectrum": the user can choose to use every level defined in the "composition.in" file (see section 3.2 below) or a limited number only. The same thing is possible for spectral narrowband intervals. The code can check reference spectra files do contain information for the required spectral region, but this test takes a lot of time and can be disabled if you are sure the required spectral data is available. Finally, the user should indicate whether or not GAS MIX has to produce the k-distribution data sets associated with interpolated high-resolution spectra. In the case the k-distribution have to be computed, GAS MIX will use the narrowband spectral limits that are defined within the "narrowbands.in" file (see section 3.2 below).

- Section "Production of quadrature and k-distributions": when the computation of k-distributions is required, the user can choose among several quadrature types. See notes at the end of the "options.in" file

for available quadrature types (the user can also use his own quadrature abscissas and weights). The quadrature order has to be specified, and additional data is required for particular quadrature types. Additionnal data may be specified, such as the size of acceleration arrays, the relative error over g when inverting g(k(i)), and whether linear or cubic spline interpolation has to be used over discrete interpolated high-resolution spectra (this depends on the accuracy of the spectral discretization used when computing reference high-resolution spectra with KSPECTRUM).

3.2   Other input files

3.2.1   Atmospheric composition

is provided via the "data/composition.in". This file must contain a label for the atmospheric composition, the number of atmospheric levels, the number of molecular species, the label of each molecular species, and, for each atmospheric level: altitude in km (unused at present date), pressure in atm, temperature in Kelvin, and the molar fraction (or partial pressure) of each molecular species. See the example file that should be produced at installation.

Molecule labels have to be identical to labels used in the HITRAN nomenclature. Labels of molecules defined in the HITRAN database can be found in the "data/molparam*.txt" file. They are obvious for most species: "H2O" is used for water vapor, "CO2" for carbon dioxide, etc. Please use capital letters when providing molecule labels in the "data/composition.in" file, and note that molecule labels must be provided between brackets (example: "$[H_2O]$") so that the code can identify molecular species.

3.2.2   Narrowband intervals

have to be provided in the "data/narrowbands.in" file, provided that the user chose to use a pre-defined narrowband discretization (see section 3.1). This file must contain the number of narrowband intervals, and, for each interval, its lower and upper limits, in terms of wavenumber (in cm^{-1}).

3.3   Running GAS MIX

Once everything is installed and the executable file "gas_mix.exe" file has been compiled, you can try to run a computation. I would recommend that, for the first time, you run GAS MIX over a single atmospheric level, for a limited number of narrowband intervals, using a simple atmospheric composition (the provided example composition for instance).

Use the following command to run the code:

> ./gas_mix.exe

4 Results

4.1 Results files

GAS MIX will produce results files in the "results" directory:

4.1.1 Interpolated high-resolution spectra:

there is one file per atmospheric level. Files are named "k***" with "***" the index of the atmospheric level. For instance, "results/k001" is the result file produced for the first atmospheric level that is defined within the "data/composition.in" file.

Each file contains 3 columns. The fist column gives values of wavenumbers, in cm^{-1}. The second column is the total cross-section of the gas mixture (in $cm^2/molecule$), at the corresponding wavenumber. The third column is the total absorption coefficient (in m^{-1}) at the corresponding wavenumber.

4.1.2 K-distribution data sets:

are located within the "results/kdist.txt" file. For each (P,T) level, k-distribution data is provided on the basis of one line per narrowband interval. For each line, the spectral limits of the interval are given, then the "Nq" values of k are provided; the last value is the relative error between the transmittivity of a 1-meter column of gas computed using the k-distribution data and computed using the discretized interpolated high-resolution spectrum (value is -1 when irrelevant, which is OK). The quality of the k-distribution data set is recorded into the "results/quadrature_results.txt" file: information is provided on the quality of the quadrature weights and on the ability of the k-distribution data set to compute the moments of the distribution.

4.2 More output files

Additionally, the user can check a number of log files produced by GAS MIX during its execution:

- "log/log_[mol]lev[i]": information about reference high-resolution spectra that have been used in order to interpolate the spectrum for molecular species [mol], at level [i].

- "results/k[mol]_lev[i]": interpolated spectrum for molecular species [mol], at level [i].