JURASSIC - High-Q

SimLab Climate, JSC, FZJ, Jülich, Germany [1]

29th July 2014

[1]Contact: l.hoffmann@fz-juelich.de, s.griessbach@fz-juelich.de

Contents

1 Introduction

The Juelich Rapid Spectral Simulation Code (JURASSIC) is a fast radiative transfer model for the mid-infrared spectral region (Hoffmann, 2006). It was used in several studies for the infrared limb sounder Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) (Hoffmann et al., 2005, 2008), Cryogenic Infrared Spectrometers and Telescopes for the Atmosphere - New Frontiers (CRISTA-NF) (Hoffmann et al., 2009; Weigel et al., 2010), and Gimballed Limb Observer for Radiance Imaging of the Atmosphere (GLORIA) (Ungermann et al., 2010) and the nadir instrument Atmospheric Infrared Sounder (AIRS) (Hoffmann and Alexander, 2009; Grimsdell et al., 2010; Hoffmann et al., 2013).

For fast simulations, it applies pre-calculated look-up tables of spectral emissivities and approximations to radiative transfer calculations, such as the emissivity growth approximation (EGA) (Weinreb and Neuendorffer, 1973; Gordley and Russell, 1981; Marshall et al., 1994).The look-up-tables were calculated with the Reference Forward Model (RFM) (Dudhia et al., 2002; Dudhia, 2014), which is an exact line-by-line model specifically developed for MIPAS. For selected spectral windows, JURASSIC has been compared to the line-by-line models RFM and Karlsruhe Optimized and Precise Radiative transfer Algorithm (KOPRA) (Stiller, 2000; Stiller et al., 2002; Höpfner and Emde, 2005) and shows good agreement (Griessbach et al., 2013).

JURASSIC contains a scattering module that allows for radiative transfer simulations including single and multiple scattering on aerosol and cloud particles (Grießbach, 2012; Griessbach et al., 2013). Forward simulations with scattering on volcanic ash, ice and sulfate aerosol have been used to develop and characterise a volcanic ash detection method for MIPAS (Griessbach et al., 2012, 2014).

Retrieval of large satellite data sets (e.g. AIRS) require plenty of computing time that can be provided by supercomputers. JURASSIC works on JUROPA and JUQUEEN at the Jülich Supercomputing Centre (JSC), Forschungszentrum Jülich GmbH (Hoffmann, 2014).

This documentation is neither ready nor perfect, but it is a start to introduce you to JURASSIC and to enable you to work and to do science with this code package.

2 Getting Started

2.1 Quick Start

The following description is for Linux users. To download the code you have to apply for an account. First, register here:

`https://cst.version.fz-juelich.de/`

and second, send us an e-mail with your username. We will activate your account.
`s.griessbach@fz-juelich.de` or
`l.hoffmann@fz-juelich.de`

You can either download the code as a .zip (.tar) file or use git clone. For the git clone move to the directory where you want to put the code and type:

```
git clone git@cst.version.fz-juelich.de:climate/jurassic.git
```

This will create the directory `jurassic` with the following subdirectories: `clim`, `docu`, `examples`, `lib`, `refrac`, `src`.

Go to `src` and run the Makefile. If it finishes without error, go to `examples` run `clear.sh`, `aero0.sh` and `aero1.sh`. If this works you're done and you can start your own projects.

```
cd src
make
cd ../examples
clear.sh
aerosol0.sh
aerosol1.sh
```

If the makefile does not finish without any error either the paths to the GSL and/or NetCDF libraries are wrong or the libraries are not installed. Install the libraries and/or add the library and include paths to the makefile. If this does not work or if there are any other problems, please contact `s.griessbach@fz-juelich.de` or `l.hoffmann@fz-juelich.de`.

2.2 JURASSIC Repository

The JURASSIC repository contains 6 folders:

folder	content
`clim`	climatology data from Remedios et al. (2007)
`docu`	this documentation
`examples`	example setups
`lib`	scripts to install the required GSL and NetCDF libraries (if required)
`refrac`	selection of refractive indices for scattering simulations
`src`	JURASSIC source files

The JURASSIC source code is written in C and we usually compile the code with the GCC. The code only requires the GSL and NetCDF libraries. In case the libraries are not installed and you do not have root access you can install the packages provided in `lib`.

2.3 How to do ...? - Examples

The following examples will show you how to use the JURASSIC modules, to do various forward simulations and retrievals. The detailed documentation of the JURASSIC modules is given in Section 5. For each example the required input files and output files are listed. The detailed descriptions of input and output files are given in Sections 3 and 4. The most substantial input file is the control file (Section 3.3). It contains all flags to setup the runs. We try to demonstrate the usage of all flags in the examples. The examples discussed here you will find in the `examples` folder as working examples.

2.3.1 Limb Clear Air Forward Simulation

Input files:

- clear-air.ctl: control file with global control flags
- atm.tab: atmospheric profile created for polar winter atmosphere
- obs.tab: observation geometry created for limb observer for 10 tangent altitudes
- *.tab: emissivity tables for each trace gas
- *.filt: filter functions for each spectral window

Output file:

- rad.tab: forward simulation results output file name

For this example we use the `climatology` and the `limb` module to create the required atmosphere and observation file, respectively. The forward simulation is started with the `formod` module.

```
#! /bin/bash

# path
src=../src

echo "Create atmosphere..."
$src/climatology clear-air.ctl - atm.tab CLIMZONE pwin|| exit

echo "Create observation geometry..."
$src/limb clear-air.ctl 800 5 15 1 obs.tab || exit

echo "Call forward model..."
$src/formod clear-air.ctl obs.tab atm.tab rad_clear.tab || exit
```

2.3.2 Nadir Aerosol Forward Simulation

Input files:

- aerosol0.ctl: control file with global control flags
- atm.tab: atmospheric profile created for polar winter atmosphere
- obs_nadir.tab: observation geometry created for nadir observer
- *.tab: emissivity tables for each trace gas
- *.filt: filter functions for each spectral window
- aero0.tab: aerosol/cloud geometry and microphysical properties
- complex refractive index file as given in aero.tab

Output file:

- rad_aero0.tab: forward simulation results output file name

For this example we use the `climatology` and the `nadir` module to create the required atmosphere and observation file, respectively. The forward simulation is started with the `formod` module.

```bash
#! /bin/bash

# path
src=../src

echo "Create atmosphere..."
$src/climatology aerosol1.ctl - atm.tab CLIMZONE pwin || exit

echo "Create observation geometry..."
$src/nadir aerosol1.ctl 800 0 10 1 obs_nadir.tab || exit

echo "Call forward model..."

$src/formod aerosol0.ctl obs_nadir.tab atm.tab rad_aero0.tab \
            AEROFILE aero0.tab|| exit
```

2.3.3 Limb Aerosol Forward Simulation

Input files:

- aerosol1.ctl: control file with global control flags
- atm.tab: atmospheric profile created for polar winter atmosphere
- obs.tab: observation geometry created for nadir observer
- *.tab: emissivity tables for each trace gas
- *.filt: filter functions for each spectral window
- aero1.tab: aerosol/cloud geometry and microphysical properties
- complex refractive index file as given in aero.tab

Output file:

- rad_aero1.tab: forward simulation results output file name

For this example we use the `climatology` and the `limb` module to create the required atmosphere and observation file, respectively. The forward simulation is started with the `formod` module.

```bash
#! /bin/bash

# path
src=../src

echo "Create atmosphere..."
$src/climatology aerosol1.ctl - atm.tab CLIMZONE pwin || exit

echo "Create observation geometry..."
$src/nadir aerosol1.ctl 800 0 10 1 obs.tab || exit

echo "Call forward model..."

$src/formod aerosol1.ctl obs_nadir.tab atm.tab rad_aero1.tab \
            AEROFILE aero1.tab|| exit
```

2.3.4 Limb Clear Air Retrieval

- .ctl: control file with global control flags
- atm.tab: atmospheric profiles/mixing ratios
- obs.tab: observations and geometry
- rad.tab: forward simulation results output file name ???
- tables
- measurement data converted to obs.tab
- maybe one example for clear air nadir
- another example for clear air limb

3 Input Files

3.1 Aerosol File

The aerosol file (`aero.tab`) contains a single 1D cloud scenario with the parameters given in Table 1. An aerosol scenario can be composed of multiple aerosol models. Each aerosol model contains data for a single scattering model in a single layer. The aerosol data must be given sorted starting with the highest layer and ending with the lowest layer. Please make sure that the layers, including their transition layers, do not overlap. Multiple cloud models can be superposed within one layer (e.g. multi-modal lognormal size distribution, different refractive indices, different scattering models). For this, please make sure that top and bottom altitudes are exactly the same. An example is given below.

Table 1: *Columns of `aero.tab` file*

# $1	=	aerosol layer top altitude [km]
# $2	=	aerosol layer bottom altitude [km]
# $3	=	transition layer thickness [km]
# $4	=	source for optical properties
# $5	=	refractive index file
# $6	=	particle concentration of log-normal mode in cm^{-3}
# $7	=	median radius of log-normal mode in μm
# $8	=	width of log-normal mode

Do:

```
14.0  13.0  0.01  MIE  ../refrac/ice-266K-warren.dat     0.032  3.6    1.6
14.0  13.0  0.01  MIE  ../refrac/h2so4-215K-shettle.dat  340.0  0.065  1.7
14.0  13.0  0.01  MIE  ../refrac/h2so4-215K-shettle.dat  5.0    0.49   1.3
12.0  10.0  0.01  MIE  ../refrac/h2so4-215K-shettle.dat  340.0  0.065  1.7
12.0  10.0  0.01  MIE  ../refrac/h2so4-215K-shettle.dat  5.0    0.49   1.3
9.0    8.0  0.01  MIE  ../refrac/ice-266K-warren.dat     0.032  3.6    1.6
```

Don't:

```
14.0  13.0  0.01  MIE  ../refrac/ice-266K-warren.dat     0.032  3.6    1.6
14.0  13.0  0.01  MIE  ../refrac/h2so4-215K-shettle.dat  340.0  0.065  1.75
14.0  12.0  0.01  MIE  ../refrac/h2so4-215K-shettle.dat  5.0    0.49   1.3
```

Column 3, the transition layer thickness, defines the distance where the particle concentration decreases to zero. We highly recommend to use sharp cloud edges or small transition layers e.g. 0.01 km.

Column 4, the source for the optical properties can be

- Mie: internal Mie code with Gauss-Hermite integration
- Ext: external database, e.g. for non-spherical particles *not implemented yet*

Column 5 contains the path and name of an external file. For the Mie code complex refractive indices are required. The refractive index file is described in 3.7. For an external database of optical properties the file name must be given here. The optical properties database format is described in 3.6.

Columns 6 – 8, for Mie calculations we use mono-modal log-normal particle size distributions with the parameters (particle concentration, median radius and width) given in columns 6 to 8. If an external database is used columns 6 to 8 must be set to "0".

The aerosol/cloud and scattering related control file parameters are listed in Table 3.

Sabines hint:
Generally transition layers are a nasty idea. They make physical interpretations much more difficult, e.g see Griessbach et al. (2013) and Höpfner et al. (2009) scenarios 4 and 5 for the effects of transition layer sampling. I strongly recommend to avoid large transition layers as long as possible.

Anyway, real clouds usually have sharp cloud edges (e.g. lifting condensation level).

3.2 Atmosphere File

The atmosphere file (`atm.tab`) is a XX+1 column list containing the temperature, pressure and volume mixing ratio profiles on a certain altitude grid. The number of total columns increases with the number of trace gases. The column order of the trace gases must be the same as the trace gas name order given in the control file (3.3). The programme `climatology` (5.1.2) can be used to generate some default atmosphere files with an arbitrary altitude grid. The atmosphere related control file parameters are listed in Table 3.

The atmosphere file is the setup information for forward simulations. For retrievals it is the a priori information. Retrieval results are written in the same format (atmosphere structure) into a new file (e.g `atm_res.tab`). The retrieval output file names are hard-coded.

Table 2: Columns of `atm.tab` *file*

# $1	=	time (seconds since 2000-01-01T00:00Z)
# $2	=	altitude [km]
# $3	=	longitude [deg]
# $4	=	latitude [deg]
# $5	=	pressure [hPa]
# $6	=	temperature [K]
# $7	=	CO2 volume mixing ratio
# $8	=	H2O volume mixing ratio
# $9	=	O3 volume mixing ratio
# $XX	=	XX volume mixing ratio
# $XX+1	=	window 0: extinction [1/km]

3.3 Control File

The control file (e.g. `clear.ctl`) contains all general setup parameters for simulation and retrieval runs. All mandatory and optional parameters are listed in Tables 3 and 4. Examples for clear air and aerosol simulation setups can be found in the `examples` folder.

3.3.1 Aerosol and Clouds

To include scattering on aerosol and cloud particles into the simulations up to 15 scattering models can be used. One scattering model can be a single mode of a multi-modal size distribution. To simulate a three modal size distribution three scattering models must be used (and placed at the same altitude in the aerosol input file). For each model individual refractive indices may be used. It is also possible to combine Mie-scattering and external databases in the same aerosol/cloud layer. For a clear air simulation the number of scattering model must be set to 0.

It is also possible to define an aerosol/cloud scenario and to neglect the scattering by setting the multiple scattering flag to 0. In this case you can choose if you want to use either the absorption or the extinction coefficient of the aerosol/cloud layers. (See Höpfner and Emde (2005) to learn which is best for a particular scenario.)

For a single scattering simulation the multiple scattering flag must be set to 1. If it is set to 2 or larger multiple scattering is simulated by also scattering the incoming rays that are calculated for the scattering source term.

Table 3: *Control flags*

flag name	purpose	default	options
Emitter			
NG EMITTER[NG]	number of emitter emitter name (trace gas name)	0 " "	0 − 15 List of emitter names in Section 3.3.4
Radiance channels			
ND NU[ND]	number of radiance channels central wave number of each channel in cm^{-1}	0 " "	0 − 50 range: 600 − 3000 cm^{-1} ???
Spectral windows			
NW	number of spectral windows	1	1 − 5
WINDOW[ND]	window index of each channel	0	
Emissivity look-up tables			
TBLBASE	look-up table path and prefix	"-"	
Hydrostatic equilibrium			
HYDZ	reference height for hydrostatic pressure profile	-999	-999: skip this option in km???
Continua			
CTM_CO2 CTM_H2O CTM_N2 CTM_O2	CO2-continuum H2O-continuum N2-continuum O2-continuum	1 1 1 1	0: off; 1: on 0: off; 1: on 0: off; 1: on 0: off; 1: on
Aerosol and Clouds			
SCA_N	number of scattering models	0	0 − 15 0: clear air (no extinction, no scattering)
SCA_MULT	multiple scattering - number of recursions; to be used if SCA_N≥1	1	0: extinction only 1: single scattering ≥2: multiple scattering
SCA_EXT	extinction coefficient; to be used if SCA_MULT= 0	beta_a	beta_e: β_e beta_a: β_a
Atmosphere/Climatology			
ZMIN ZMAX DZ	atmosphere bottom altitude atmosphere top altitude atmosphere vertical grid	0 0 1	in km in km in km

Table 4: *Control flags*

flag name	purpose	default	options
Ray-tracing			
REFRAC	refraction in the atmosphere	1	1: on; 0: off
RAYDS	maximum step lengths for raytracing	10	10 km: suitable for limb 1 km: suitable for nadir
RAYDZ	maximum vertical component of step length	1	1 km is reasonable
TRANSS	transition layer sampling step	0.02	0.01-0.1 km is reasonable
Interpolation of atmospheric data			
IP	interpolation method	1	1: profile 2: satellite track 3: Lagrangian grid
CZ	influence length for vertical interpolation	0	in km
CX	influence length for horizontal interpolation	0	in km
Field of view			
FOV	field-of-view data file	"-"	path+filename
Retrieval interface			
RETP_ZMIN	minimum altitude for pressure retrieval	-999	in km
RETP_ZMAX	maximum altitude for pressure retrieval	-999	in km
RETT_ZMIN	minimum altitude for temperature retrieval	-999	in km
RETT_ZMAX	maximum altitude for temperature retrieval	-999	in km
RETQ_ZMIN[NG]	minimum altitude for volume mixing ratio retrieval	-999	in km
RETQ_ZMAX[NG]	maximum altitude for volume mixing ratio retrieval	-999	in km
RETK_ZMIN[NW]	minimum altitude for extinction retrieval	-999	in km
RETK_ZMAX[NW]	maximum altitude for extinction retrieval	-999	in km
Output flags			
WRITE_BBT	use brightness temperature instead of radiance	0	0: no; 1: yes
WRITE_MATRIX	write matrix data	0	0: no; 1: yes

3.3.2 Continua

TO DOkurze Beschreibung, welches Schema?

3.3.3 Emissivity look-up Tables

Basename for table files and filter function files. Look-up tables are created in instrument specific spectral resolution/sampling. The look-up tables are described in 3.8.

3.3.4 Emitter

A list of supported trace gases is given in Table 5. The reading routine is not case sensitive.

3.3.5 Field of View

TO DO

3.3.6 Ray-tracing

The lengths of the line-of-sight segments to be integrated is either determined by RAYDS (total segment length) or RAYDZ (z-component of segment length). For limb scenarios RAYDS is most likely the limiting value and in nadir scenarios RAYDZ will be the limiting value. For limb-scenarios RAYDS = 10 km is reasonable. In nadir and sub-limb-scenarios a segment length of 10 km is too much to sample steep atmospheric gradients (temperature, trace gases). Especially for scattering simulations, where limb, sub-limb and nadir paths are calculated a reasonable combination of RAYDS and RAYDZ is required for fast and accurate simulations. From our experience RAYDS = 10 km and RAYDZ = 0.1 − 1 km offer a good trade off for accuracy and efficiency.

For cloud and aerosol simulations with a transition layer larger than 20 m the parameter TRANSS refines the sampling grid within the transition layer. The default value is TRANS = 20 m. (Please see further comments on raytracing and transition layers in Section 5.2.6.)

Table 5: *Trace Gases*

Emitter Name	Formula	Name
C2H2	C_2H_2	acetylene
C2H6	C_2H_6	ethane
CCl4	CCl_4	carbon tetrachloride
CH4	CH_4	methane
ClO	ClO	chlorine monoxide
ClONO2	$ClONO_2$	chlorine nitrate
CO	CO	carbon monoxide
COF2	COF_2	carbonyl fluoride
F11	CCl_3F	trichlorofluoromethane
F12	CCl_2F_2	dichlorodifluoromethane
F14	CF_4	tetrafluoromethane
F22	$CHClF_2$	chlorodifluoromethane
H2O	H_2O	water
H2O2	H_2O_2	hydrogen peroxide
HCN	HCN	hydrogen cyanide
HNO3	HNO_3	nitric acid
HNO4	HNO_4	peroxynitric acid
HOCl	HOCl	hypochlorous acid
N2O	N_2O	nitrous oxide
N2O5	N_2O_5	dinitrogen pentoxide
NH3	NH_3	ammonia
NO	NO	nitric oxide
NO2	NO_2	nitrogen dioxide
O3	O_3	ozone
OCS	OCS	carbonyl sulfide
SF6	SF_6	sulfur hexafluoride
SO2	SO_2	sulfur dioxide

3.3.7 Spectral Windows

Each channel can be assigned to a window e.g. to have a constant extinction for all channels.

3.4 Directory List

TO DO

3.5 Observation File

The observation file (`obs.tab`) is a multi-column list containing the geometry information (time, observer, view point and tangent point position) and the (measured) radiances (and/or transmittances) for each channel. (View point and tangent point differ, because of atmospheric refraction.) The number of columns increases with the number of channels. For retrievals this file contains the measurements. For forward simulations this file defines the viewing geometry. Columns 1 to 7 are mandatory. The forward simulation output is written in the same format (observation structure) into a new file specified when calling the forward model (e.g. `rad.tab`). The JURASSIC modules `limb` and `nadir` (Section 5.1.7 and 5.1.8) can be used to create an observation geometry.

Table 6: *Columns of `obs.tab` file*

# $1	=	time [seconds since 2000-01-01T00:00Z]
# $2	=	observer altitude [km]
# $3	=	observer longitude [deg]
# $4	=	observer latitude [deg]
# $5	=	view point altitude [km]
# $6	=	view point longitude [deg]
# $7	=	view point latitude [deg]
# $8	=	tangent point altitude [km]
# $9	=	tangent point longitude [deg]
# $10	=	tangent point latitude [deg]
# $11	=	channel 792: radiance [W/(m^2 sr cm^{-1})]
# $12	=	channel 792: transmittance
# $XX	=	channel XX: radiance [W/(m^2 sr cm^{-1}]
# $XX+1	=	channel XX: transmittance

3.6 Optical Properties Database

TO DONot implemented yet.

3.7 Refractive Index File

The refractive index file contains the wavenumber dependent complex refractive indices in the format given in Table 7. A formatted collection can be found in the folder `refrac`. One file contains the data set for one temperature (given in the file name).

All refractive indices are taken from the HITRAN database (Rothman et al., 2009) aerosol compilation. References to the original sources are given there.

Table 7: *Columns of the refractive index files*

# $1	=	wavenumber [cm-1]
# $2	=	real part
# $3	=	imaginary part

3.8 Tables

TO DODescribe me!!!

4 Output Files

rad.tab, same structure as observation file

Table 8: *Columns of `rad.tab` file*

# $1	=	time [seconds since 2000-01-01T00:00Z]
# $2	=	observer altitude [km]
# $3	=	observer longitude [deg]
# $4	=	observer latitude [deg]
# $5	=	view point altitude [km]
# $6	=	view point longitude [deg]
# $7	=	view point latitude [deg]
# $8	=	tangent point altitude [km]
# $9	=	tangent point longitude [deg]
# $10	=	tangent point latitude [deg]
# $11	=	channel 792: radiance [W/(m^2 sr cm^{-1})]
# $12	=	channel 792: transmittance
# $XX	=	channel XX: radiance [W/(m^2 sr cm^{-1}]
# $XX+1	=	channel XX: transmittance

5 JURASSIC Modules and Libraries

5.1 Modules

5.1.1 brightness

The `brightness` programme calculates the brightness temperature in K for a given radiance in W/(m^2 sr cm^{-1}) and wave number in cm^{-1}.

Example

```
../src/brightness [radiance] [wavenumber]
../src/climatology 0.0231451 960
```

5.1.2 climatology

The `climatology` programme can be used to generate the atmosphere file (`atm.tab`). This programme interpolates the chosen climatology from Remedios et al. (2007) onto the defined altitude grid and adds the trace gases in the same order as given in the control file. One can choose between polar winter (pwin), polar summer (psum), midlatitude (midl) and equatorial (equ) atmosphere (example line 3). The default is the midlatitude atmosphere (example line 2). The input grid can be taken from an already existing `atm.tab` file (example line 4). The grid points e.g. with 500 m vertical spacing will be taken from the file, but not the data! The control file parameters relevant for the climatology module can be found in Table 3 in the Emitter and Atmosphere/Climatology sections.

The Remedios climatology `clim_remedios.tab` is in the `clim` folder. Either copy the climatology into the working directory or set a link.

Examples

```
1 ../src/climatology [control file] [input grid] [output] [optional]
2 ../src/climatology clear-air.ctl - atm.tab
3 ../src/climatology clear-air.ctl - atm.tab CLIMZONE pwin
4 ../src/climatology clear-air.ctl atm2.tab atm.tab
```

5.1.3 collect

TO DO

5.1.4 formod

The `formod` module is the programme that starts a forward simulation. The minimum required input are the control file (Section 3.3), the observation file (Section 3.5), the atmosphere file (Section 3.2) and the output file (Section 4).

Optional are TASK, DIRLIST (Section 3.4) and AEROFILE (Section 3.1). The option TASK c calculates the contribution of each specified trace gas separately. How are the results stored? TO DO

The option DIRLIST provides a file with directories. Each directory must contain a control file, observation file, atmosphere file and optionally an aerosol file with the same name, but different content. The DIRLIST is a feature that is used to distribute large simulation/retrieval sets among multiple cores, e.g. on a supercomputer.

The option AEROFILE is required for scattering simulations. The AEROFILE contains the aerosol/cloud altitude information and the corresponding microphysical cloud/ aerosol properties.

Examples

```
../src/formod [control file] [observation file] [atmosphere file] \
              [output]
../src/formod clear-air.ctl obs.tab atm.tab rad.tab
../src/formod clear-air.ctl obs.tab atm.tab rad.tab TASK c
../src/formod clear-air.ctl obs.tab atm.tab rad.tab \
              DIRLIST dirlist-orbit.asc
../src/formod aerosol1.ctl obs.tab atm.tab rad.tab AEROFILE aero.tab
../src/formod aerosol1.ctl obs.tab atm.tab rad.tab \
              DIRLIST dirlist-aero.asc AEROFILE aero.tab
```

Instead of giving TASK, DIRLIST and AEROFILE as input, it can also be specified in the control file:

```
AEROFILE = aero.tab
DIRLIST = dirlist-clim.asc
TASK = c
```

5.1.5 interpolate

TO DO

5.1.6 kernel

TO DO

5.1.7 limb

The `limb` programme creates an observation file (Section 3.5) for a specified limb geometry. In the example line 1 an observation file with 11 view point altitudes between 5 and 15 km is created.

Example

```
1 ../src/limb [control file] [observer altitude] \
2             [min view point altitude] [max view point altitude max] \
3             [delta altitude] [output]
4 ../src/limb aerosol1.ctl 800 5 15 1 obs.tab
```

5.1.8 nadir

The `nadir` programme creates an observation file (Section 3.5) for the nadir geometry. In the example line 1 an observation file with nadir trace consisting of 11 points from 0 to 10 N is created.

Example

```
1 ../src/nadir [control file] [observer altitude] [min latitude] \
2              [max latitude] [delta latitude] [output]
3 ../src/nadir aerosol1.ctl 800 0 10 1 obs_nadir.tab
```

5.1.9 planck

The `planck` programme returns the Planck radiance in W/(m^2 sr cm$^-$1) for a given temperature in K and wavenumber in cm^{-1}.

Example

```
1 ../src/planck [temperature] [wavenumber]
2 ../src/planck 270 960
```

5.1.10 raytrace

The `raytrace` programme can be used to perform the raytracing for a given geometry in a given atmosphere and to dump out the line of sight points and certain diagnostics into the files `raytrace.tab` and `los.0`. Further input options are: LOSBASE, MASSBASE and AEROFILE.

AEROFILE in example line 4 includes an aerosol file, so that the fine sampling around the aerosol/cloud edges is included into the raytracing. (see Section 5.2.6

LOSBASE creates the output file `los.0` if no other name is specified. It is switched on by default. In example line 6 the output file `liofsi.0` is created. Example line 7 shows how to switch it off.

MASSBASE in example line 8 creates the output files `mass.numdens.0` and `mass.coldens.0`. TO DOwhat is in these files?

Examples

```
1 ../src/raytrace [control file] [observer file] [atmosphere file] \
2                 [options]
3 ../src/raytrace clear-air.ctl obs_raytrace.tab atm.tab
4 ../src/raytrace clear-air.ctl obs_raytrace.tab atm.tab \
5                 AEROFILE aero1.tab
6 ../src/raytrace clear-air.ctl obs_raytrace.tab atm.tab LOSBASE liofsi
7 ../src/raytrace clear-air.ctl obs_raytrace.tab atm.tab LOSBASE -
8 ../src/raytrace clear-air.ctl obs_raytrace.tab atm.tab MASSBASE mass
```

5.1.11 retrieval

TO DO

5.1.12 tab2bin

The `tab2bin` programme can be used to convert the ASCII tables to binary format. Using binary format tables significantly reduces the file I/O time during e.g. `formod` runs. This programme should be run on the architecture where the JURASSIC programmes using these tables will be executed. Please note, tables converted on JUROPA cannot be used on JUQUEEN and vice versa.

Example

```
../src/tab2bin [control file]
../src/tab2bin clear_air.ctl
```

5.2 Libraries

5.2.1 atmosphere.h/c

contains routines that deal with atmospheric data, atmospheric composition

5.2.2 continua.h/c

contains routines to calculate CO_2, H_2O, N_2 and O_2 continua

5.2.3 control.h/c

contains routines to read and scan the control file

5.2.4 forwardmodel.h/c

contains functions relevant to the forward model, radiative transfer calculation, table interpolation,...

5.2.5 jurassic.h

contains macros, constants (Appendix A.1), dimensions (Appendix A.2), and global struct definitions

5.2.6 lineofsight.h/c

contains functions that deal with raytracing and the line of sight Aerosol and cloud sampling: Done in raytracing. Extra los points about 5 m above and below cloud edges.

5.2.7 retrievalmodel.h/c

contains functions that deal with the retrieval

5.2.8 scatter.h/c

contains routines concerning scattering on aerosol and clouds; mie scattering is following Bohren and Huffman (1983) code; Gauss-Hermite scheme used for integration over log-normal size distribution; scattering of solar radiation included

5.2.9 sonstige.h/c

contains routines that are used by several other programmes and routines

5.3 Makefile

A Lists of Constants and Dimensions

A.1 Physical Constants

Table 9: *Physical constants in* `pirat.h`*.*

name	purpose	value
C1	First spectroscopic constant ($c_1 = 2hc^2$) [W/(m^2 sr cm^{-4})]	1.19104259e-8
C2	Second spectroscopic constant ($c_2 = hc/k$) [K/cm^{-1}]	1.43877506
P0	Standard pressure [hPa]	1013.25
RE	Mean radius of Earth [km]	6367.421
ME	Mass of Earth [kg]	5.976e24
SCA_TSUN	temperature of the sun [K]	5780

A.2 Dimensions

Table 10: *Dimensions in `control.h`.*

name	purpose	value
LEN	Maximum length of ASCII data lines	5000
MMAX	Maximum size of measurement vector	(NRMAX×NDMAX)
NMAX	Maximum size of state vector	(NQMAX×NPMAX)
NQMAX	Maximum number of quantities	(2+NGMAX+NWMAX)
NWMAX	Maximum number of spectral windows	5
NDMAX	Maximum number of radiance channels	50
NGMAX	Maximum number of emitters	15
NLOS	Maximum number of LOS points	1000
NPMAX	Maximum number of atmospheric data points	1000
NRMAX	Maximum number of ray paths	1000
NSHAPE	Maximum number of shape function grid points	10000
NFOV	Number of ray paths used for FOV calculations	5
TBLNPMAX	Maximum number of pressure levels in emissivity tables	40
TBLNSMAX	Maximum number of source function temperature levels	1201
TBLNTMAX	Maximum number of temperatures in emissivity tables	30
TBLNUMAX	Maximum number of column densities in emissivity tables	320
SCAMOD	Maximum number of scattering models	15
NLMAX	Maximum number of aerosol/cloud layers	10
NRAD	Number of points for Gauss-Hermite integration	170
NTHETA	Number of scattering angles (from 0 to 180 deg)	181
REFMAX	Maximum number of refractive indices	5000

References

C. F. Bohren and D. R. Huffman. *Absorption and Scattering of Light by Small Particles.* John Wiley & Sons, Ltd., 1983.

A. Dudhia. *RFM Software User's Manual.* Department of Atmospheric, Oceanic and Planetary Physics, University of Oxford, United Kingdom, 2014. URL `http://www.atm.ox.ac.uk/{RFM}`. last access: 24.07.2014.

Anu Dudhia, Paul E. Morris, and Robert J. Wells. Fast monochromatic radiative transfer calculations for limb sounding. *J. Quant. Spectrosc. Radiat. Transfer*, 74: 745–756, 2002.

Larry L. Gordley and James M. Russell. Rapid inversion of limb radiance data using an emissivity growth approximation. *Appl. Optics*, 20:807–813, 1981.

S. Griessbach, L. Hoffmann, M. von Hobe, R. Müller, R. Spang, and M. Riese. A six-year record of volcanic ash detection with Envisat MIPAS. In *Proceedings of ESA ATMOS 2012*. European Space Agency, ESA Special Publication SP-708 (CD-ROM), 2012.

S. Griessbach, L. Hoffmann, M. Hoepfner, M. Riese, and R. Spang. Scattering in infrared radiative transfer: A comparison between the spectrally averaging model JURASSIC and the line-by-line model KOPRA. *J. Quant. Spectrosc. Radiat. Transfer*, 27:102–118, 2013. doi: 10.1016/j.jqsrt.2013.05.004.

S. Griessbach, L. Hoffmann, R. Spang, and M. Riese. Volcanic ash detection with infrared limb sounding: MIPAS observations and radiative transfer simulations. *Atmos. Meas. Tech.*, 7(5):1487–1507, 2014. doi: 10.5194/amt-7-1487-2014.

Sabine Grießbach. *Clouds and aerosol in infrared radiative transfer calculations for the analysis of satellite observations*, volume 139 of *Schriften des Forschungszentrums Jülich, Reihe Energie & Umwelt.* Forschungszentrum Jülich, Jülich, 2012. ISBN 978-3-89336-785-6. URL `http://juwel.fz-juelich.de:8080/dspace/handle/2128/4597`. last access: 24.07.2014.

Alison W. Grimsdell, M. Joan Alexander, Peter T. May, and Lars Hoffmann. Model study of waves generated by convection with direct validation via satellite. *J. Atmos. Sci.*, 67(5):1617–1631, 2010.

L. Hoffmann, 2014. URL `http://www.fz-juelich.de/ias/jsc/EN/Expertise/High-Q-Club/JURASSIC/_node.html`. last access: 24.07.2014.

L. Hoffmann and M. J. Alexander. Retrieval of stratospheric temperatures from Atmospheric Infrared Sounder radiance measurements for gravity wave studies. *J. Geophys. Res.*, 114, 2009. doi: 10.1029/2008JD011241.

L. Hoffmann, M. Kaufmann, R. Spang, R. Müller, J.J. Remedios, D. P. Moore, C. M. Volk, T. von Clarmann, and M. Riese. Envisat MIPAS measurements of CFC-11: retrieval, validation, and climatology. *Atmos. Chem. Phys.*, 8:3671–3688, 2008.

L. Hoffmann, K. Weigel, R. Spang, S. Schroeder, K. Arndt, C. Lehmann, M. Kaufmann, M. Ern, P. Preusse, F. Stroh, and M. Riese. CRISTA-NF measurements of water vapor during the SCOUT-O3 Tropical Aircraft Campaign. *Adv. Space Res.*, 43: 74–81, 2009.

L. Hoffmann, X. Xue, and M. J. Alexander. A global view of stratospheric gravity wave hotspots located with Atmospheric Infrared Sounder observations. *J. Geophys. Res.*, 118:416–434, 2013. doi: 10.1029/2012JD018658.

Lars Hoffmann. Schnelle Spurengasretrieval für das Satellitenexperiment Envisat MIPAS. Technical Report JUEL-4207, Forschungszentrum Jülich, Germany, 2006. ISSN 0944-2952.

Lars Hoffmann, Reinhold Spang, Martin Kaufmann, and Martin Riese. Retrieval of CFC-11 and CFC-12 from Envisat MIPAS observations by means of rapid radiative transfer calculations. *Adv. Space Res.*, 36:915–921, 2005.

M. Höpfner, M. C. Pitts, and L. R. Poole. Comparison between CALIPSO and MIPAS observations of polar stratospheric clouds. *J. Geophys. Res.*, 114, 2009. doi: 10.1029/2009JD012114.

Michael Höpfner and Claudia Emde. Comparison of single and multiple scattering approaches for the simulation of limb-emission observations in the mid-IR. *J. Quant. Spectrosc. Radiat. Transfer*, 91:275–285, 2005.

Benjamin T. Marshall, Larry L. Gordley, and D. Allen Chu. BANDPAK: Algorithms for modeling broadband transmission and radiance. *J. Quant. Spectrosc. Radiat. Transfer*, 52:581–599, 1994.

J. J. Remedios, R. J. Leigh, A. M. Waterfall, D. P. Moore, H. Sembhi, I. Parkes, J. Greenhough, M.P. Chipperfield, and D. Hauglustaine. MIPAS reference atmospheres and comparisons to V4.61/V4.62 MIPAS level 2 geophysical data sets. *Atmos. Chem. Phys. Discuss.*, 7:9973–10017, 2007.

L. S. Rothman, I. E. Gordon, A. Barbe, D. C. Benner, P. E. Bernath, M. Birk, V. Boudon, L. R. Brown, A. Campargue, J. P. Champion, K. Chance, L. H. Coudert, V. Dana, V. M. Devi, S. Fally, J. M. Flaud, R. R. Gamache, A. Goldman, D. Jacquemart, I. Kleiner, N. Lacome, W. J. Lafferty, J. Y. Mandin, S. T. Massie, S. N. Mikhailenko, C. E. Miller, N. Moazzen-Ahmadi, O. V. Naumenko, A. V. Nikitin, J. Orphal, V. I. Perevalov, A. Perrin, A. Predoi-Cross, C. P. Rinsland, M. Rotger, M. Simeckova, M. A. H. Smith, K. Sung, S. A. Tashkun, J. Tennyson, R. A. Toth,

A. C. Vandaele, and J. Vander Auwera. The HITRAN 2008 molecular spectroscopic database. *J. Quant. Spectrosc. Radiat. Transfer*, 110(9-10):533–572, 2009.

G. P. Stiller. The Karlsruhe Optimized and Precise Radiative Transfer Algorithm (KOPRA). Technical Report FZKA-6487, Forschungszentrum Karlsruhe, 2000.

Gabriele P. Stiller, Thomas von Clarmann, Bernd Funke, Norbert Glatthor, Frank Hase, Michael Höpfner, and Andrea Linden. Sensitivity of trace gas abundances retrievals from infrared limb emission spectra to simplifying approximations in radiative transfer modelling. *Appl. Optics*, 41:249–280, 2002.

J. Ungermann, M. Kaufmann, L. Hoffmann, P. Preusse, H. Oelhaf, F. Friedl-Vallon, and M. Riese. Towards a 3-D tomographic retrieval for the air-borne limb-imager GLORIA. *Atmos. Meas. Tech.*, 3(4):2995–3046, 2010. doi: 10.5194/amtd-3-2995-2010.

K. Weigel, M. Riese, L. Hoffmann, S. Hoefer, C. Kalicinsky, P. Knieling, F. Olschewski, P. Preusse, F. Stroh, R. Spang, and C. M. Volk. CRISTA-NF measurements during the AMMA-SCOUT-O3 aircraft campaign. *Atmos. Meas. Tech.*, 3:1437–1455, 2010.

Michael P. Weinreb and Arthur C. Neuendorffer. Method to apply homogeneous-path transmittance models to inhomogenous atmospheres. *J. Atmos. Sci.*, 30:662–666, 1973.