JURASSIC - High-Q

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Contents

Chapter 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 (L.Hoffmann, 2014).

Chapter 2

Getting Started

2.1 Quick Start

get code from repository

(this will create directory jurassic with the subdirectories: docu, examples-tab, lib, jurassic-1.0)

run install script (check environment variables, libbuild.sh, make) (maybe one that works for JUROPA, JUQUEEN and normal workstations)

go to examples and run clear.sh

If this works you can try the other examples or start your own projects.

If any error occours, please refer to the more detailed documentation.

2.2 download the code

jurassic repository

optional/additional file repository (tables and filter functions, refractive index files, external optical properties databases, Remedios atmospheres and PSC study???)

2.3 Installation

- which libraries are needed? GSL and NCDF
- how to compile and link the code?

2.4 Code Execution

- how to run the code?
- which input is required? (link to description section)
- examples for forward simulations: clear air, aerosol scattering, retrieval

2.4.1 Forward Simulations

- .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
- *aero.tab*: aerosol and cloud parameters
- *complex refractive indices*
- or *optical properties database*
- maybe one example for clear air nadir
- another example for cloudy limb

Clear Air Simulation

```
# path
pirat=../pirat-1.0

info "Create geometry..."
$pirat/limb test.ctl 800 5 15 1 obs.tab || exit

info "Call forward model..."
$pirat/formod test-aerosol.ctl obs.tab atm.tab rad.tab || exit
```

Aerosol/Cloud Simulation

```
#£pirat/formod aerosol1.ctl obs.tab atm.tab rad.tab || exit
#£pirat/formod aerosol1.ctl obs.tab atm.tab rad.tab DIRLIST dirlist-aero.asc|| ex
$pirat/formod aerosol1.ctl obs.tab atm.tab rad.tab AEROFILE aero.tab|| exit
#£pirat/formod aerosol1.ctl obs.tab atm.tab rad.tab DIRLIST dirlist-aero.asc AERO
#£pirat/formod test.ctl obs.tab atm.tab rad.tab TASK c || exit
```

Instead of giving the filename of the aerosol data here it can also ge given in the control-file:

`AEROFILE = aero.tab`

The same holds for `DIRLIST` and `TASK`.

2.4.2 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

Chapter 3

Input Files

3.1 Aerosol File

The aerosol file (`aero.tab`) contains a single 1D cloud scenario with the parameters given in Table 3.1. 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 3.1: *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  $J/refrac/ice-266K-warren.dat     0.032  3.6    1.6
14.0  13.0  0.01  MIE  $J/refrac/h2so4-215K-shettle.dat  340.0  0.065  1.7
14.0  13.0  0.01  MIE  $J/refrac/h2so4-215K-shettle.dat  5.0    0.49   1.3
12.0  10.0  0.01  MIE  $J/refrac/h2so4-215K-shettle.dat  340.0  0.065  1.7
12.0  10.0  0.01  MIE  $J/refrac/h2so4-215K-shettle.dat  5.0    0.49   1.3
9.0    8.0  0.01  MIE  $J/refrac/ice-266K-warren.dat     0.032  3.6    1.6
```

Don't:

```
14.0  13.0  0.01  MIE  $J/refrac/ice-266K-warren.dat     0.032  3.6    1.6
14.0  13.0  0.01  MIE  $J/refrac/h2so4-215K-shettle.dat  340.0  0.065  1.75
14.0  12.0  0.01  MIE  $J/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*
- MieBin: internal Mie code with integration over binned data *not implemented yet*
- ???: we keep this extendable

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 3.6. For an external database of optical properties the file name must be given here. The optical properties database format is described in 3.5.

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 3.3.

TO DOexample for external data base

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 tool `climatology` (5.2) can be used to generate some default atmosphere files with an arbitrary altitude grid. The atmosphere related control file parameters are optional and listed in Table 3.3.

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 3.2: *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 3.3 and 3.4. Examples for clear air and aerosol simulation setups are given in Section 3.3.8.

3.3.1 Aerosol and Clouds

See Section 6.1 for detailed description.

Table 3.3: *Control flags*

flag name	purpose	default	options
Emitter			
NG	number of emitter	0	0 – 15
EMITTER[NG]	emitter name (trace gas name)	“ ”	List of emitter names in Section 3.3.4
Radiance channels			
ND	number of radiance channels	0	0 – 50
NU[ND]	central wave number of each channel in cm^{-1}	“ ”	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	CO2-continuum	1	0: off; 1: on
CTM_H2O	H2O-continuum	1	0: off; 1: on
CTM_N2	N2-continuum	1	0: off; 1: on
CTM_O2	O2-continuum	1	0: off; 1: on
Aerosol and Clouds			
SCA_N	number of scattering models	0	0 – XX 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	atmosphere bottom altitude	0	in km
ZMAX	atmosphere top altitude	0	in km
DZ	atmosphere vertical grid	1	in km

Table 3.4: *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 3.7.

3.3.4 Emitter

A list of supported trace gases is given in Table 3.5. 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 pathes 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 transition layers in Section 6.1.)

Table 3.5: *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.

3.3.8 Examples

TO DOinclude clear air and aerosol example with minted

3.4 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. (Kann mann hier statt 5-7 auch 8-10 angeben? Ist fr diese conversion im Code was vorgesehen?) 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`).

Wie generiert man eine Beobachtungsgeometrie????

Table 3.6: *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

3.5 Optical Properties Database

TO DONot implemented yet.

3.6 Refractive Index File

The refractive index file contains the wavenumber dependent complex refractive indices in the format given in Table 3.7. A formatted colletion 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 origional sources are given there.

Table 3.7: *Columns of the refractive index files*

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

3.7 Tables

TO DODescribe me!!!

Chapter 4

Output Files

output

Chapter 5

Tools

5.1 brightness

5.2 climatology

The `climatology` tool can be used to generate the atmosphere file (`atm.tab`). This tool 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 2). The default is the midlatitude atmosphere (example 1). The input grid can be taken from an already existing `atm.tab` file (example 3). 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 tool can be found in Table 3.3 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

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

5.3 collect

5.4 formod

5.5 interpolate

5.6 kernel

5.7 limb

5.8 planck

5.9 raytrace

5.10 retrieval

5.11 tab2bin

Chapter 6

Documentation

6.1 Aerosol

Aerosol and cloud sampling: Done in raytracing. Extra los points about 5 m above and below cloud edges.

Sabines hint:
Generally transition layers are a nasty idea. They make physical interpretations much more complicated/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 would strongly recommend to avoid transition layers as long as possible.

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

Appendix A

Lists of Constants and Dimensions

A.1 Physical Constants

Table A.1: *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 A.2: *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

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