

UNIVERSITY OF CENTRAL FLORIDA

Transit Users Manual

A RADIATIVE-TRANSFER CODE FOR PLANETARY
ATMOSPHERES

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1 Team Members

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2 Introduction

This document describes the University of Central Florida’s computer program `Transit`. The program calculates the transmission or emission flux spectrum of a planetary atmosphere with application to extrasolar-planet transit and eclipse observations, respectively. `Transit` calculates the spectra by solving for the 1-dimensional line-by-line radiative-transfer equation for a plane-parallel atmospheric model. A separate document (**FINDME: point to file**) describes in detail the theory and assumptions adopted by `Transit`.

This manual describes the `Transit` program usage for the user (Sections 3 through 7) and potential developer (Sections 8-9). Section 3 indicates how to obtain the code and the system requirements. Section 5 describes the inputs necessary for execution. Section 6 describes the output files produced by the code. Section 7 show an example execution of the code. Section ?? describes the program design. Sections 8 and 9 details the data structures and routines, respectively.

2.1 Transit Package Overview

`Transit` is a C code, written in a modular, object-oriented style. It was originally developed at Cornell University by Patricio Rojo, a former Ph.D. student of Dr. Joseph Harrington. The code handled the case of transmission spectrum, where stellar light is absorbed as it travels tangentially across the limb of a planetary atmosphere, as observed during an exoplanet transit observation. Subsequently, we —the exoplanet group at the University of Central Florida— have modified the code to add planetary emission spectra calculation (as observed during a secondary-eclipse observation), include multiple opacity line lists, and incorporate it to the Bayesian Atmospheric Radiative Transfer ([BART](#)²) project, which constrains exoplanet atmospheric properties in a Bayesian framework, given a set of eclipse or transit-depth measurements.

`BART` combines `Transit` with the Thermochemical Equilibrium Abundances ([TEA](#)³) module, which calculates abundances of gaseous species, and the Multi-Core Markov-chain Monte Carlo

¹<https://github.com/pcubillos/>

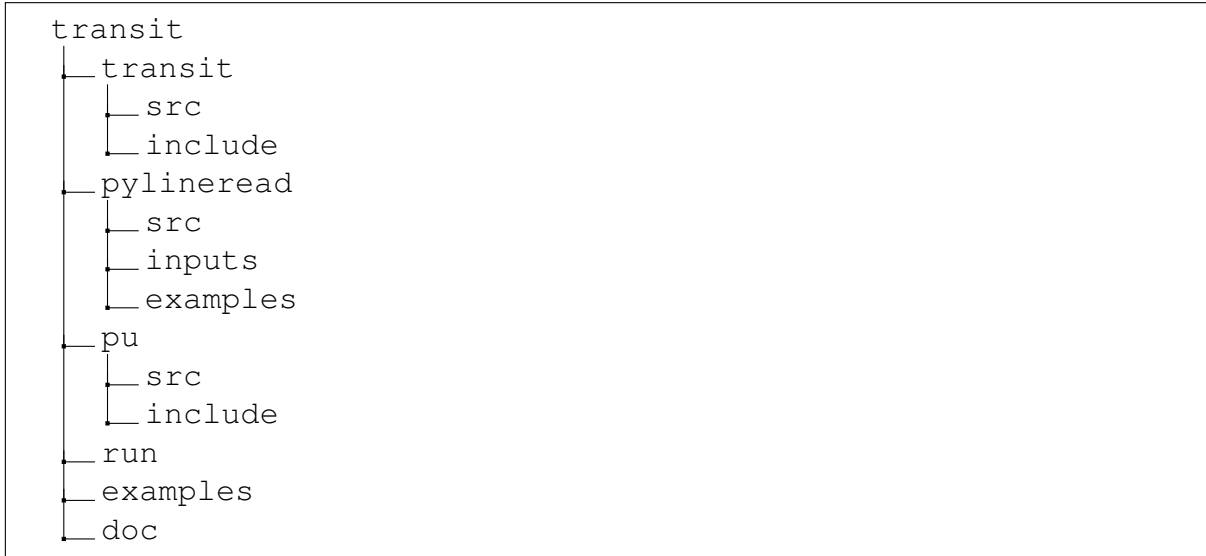
²github.com/joeharr4/BART

³github.com/dzesmin/TEA

([MCcubed](#)⁴) statistical module, which assesses the temperature and molecular-abundances posterior distributions, given a set of observations.

The current `Transit` package consists of three main modules: `Transit` (**FINDME: change name to RT**), a C module that calculates the emission or transmission spectrum for a planetary atmosphere by solving for the radiative-transfer equation. `pu`, a library of C utility functions used by `Transit`. `Pylineread`, a Python module that converts molecular line-opacity information (line transitions and partition functions) from online-available databases into the transit line information (TLI) format for later use by `Transit`.

The `Transit` module is organized as follow:



⁴github.com/pcubillos/MCcubed

2.2 License

Transit, a code to solve for the radiative-transfer equation for planetary atmospheres.

This project was completed with the support of the NASA Planetary Atmospheres Program, grant NNX12AI69G, held by Principal Investigator Joseph Harrington. Principal developers included graduate students Patricio E. Cubillos and Jasmina Blečić, programmer Madison Stemm, and undergraduate Andrew S. D. Foster. The included 'transit' radiative transfer code is based on an earlier program of the same name written by Patricio Rojo (Univ. de Chile, Santiago) when he was a graduate student at Cornell University under Joseph Harrington.

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This is a test version only, and may not be redistributed to any third party. Please refer such requests to us. This program is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.

Our intent is to release this software under an open-source, reproducible-research license, once the code is mature and the first research paper describing the code has been accepted for publication in a peer-reviewed journal. We are committed to development in the open, and have posted this code on github.com so that others can test it and give us feedback. However, until its first publication and first stable release, we do not permit others to redistribute the code in either original or modified form, nor to publish work based in whole or in part on the output of this code. By downloading, running, or modifying this code, you agree to these conditions. We do encourage sharing any modifications with us and discussing them openly.

We welcome your feedback, but do not guarantee support. Please send feedback or inquiries to:

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Thank you for using transit!

3 Installation

3.1 System Requirements

- Python.
 - NumPy.
 - mpi4py.
 - A working MPI distribution (MPICH preferred).
 - A C compiler (**FINDME: any preference?**).
 - A Fortran compiler (**FINDME: any preference?**).
 - GSL (**FINDME: give specifics**).

Transit was developed on a (**FINDME: check this**) Unix/Linux machine using Python 2.7.6, Numpy 1.8.2, and mpi4py 1.3.1. (**FINDME: Ask someone who knows about C and Fortran requirements.**)

3.2 Install and Compile

To obtain the `Transit` code download the latest stable version from the [releases⁵](#) page. Alternatively, clone the repository to your local machine with the following terminal command:

```
git clone https://github.com/pcubillos/transit transit
```

To compile the `pu` and `transit` modules execute ‘make’ on the respective folders:

```
cd transit/pu
make
cd ../transit
make
```

To compile the `pylineread` fortran code:

```
cd transit/pylineread/src/fortran
make
```

To remove the program binaries, execute (from the respective directories):

```
make clean
```

Note, there will be warnings.

⁵github.com/pcubillos/transit/releases

4 Quick Example

The following script quickly let's you calculate a methane emission spectrum:

To start, create a working directory to place the code and outputs:

```
cd
mkdir tmp/
mkdir tmp/transit_demo
cd tmp/transit_demo
```

```
cd tmp/transit_demo
```

Clone the repository to your working directory and compile the programs:

```
git clone https://github.com/pcubillos/transit transit
cd transit/puth
make
cd ../transit
make
cd ../pylineread/src/fortran
make
cd ../../../../..
```

Create a directory to place the configuration files and execute the code:

```
mkdir run
cd run
```

First we run pylineread to create a TLI file that contains the line transition data. Copy the pylineread configuration file to the run directory:

```
cp ../transit/pylineread/examples/demo/pyline_example.cfg pylane_demo.cfg
```

Download the methane line-transition database from the HITRAN server:

```
wget -user=HITRAN -password=getdata -N https://www.cfa.harvard.edu/HITRAN/HITRAN2008/HITRAN2008_H2O.zip
unzip 06_hit08.zip
```

Run pylineread:

```
../transit/pylineread/src/pylineread.py -c pylane_demo.cfg
```

Now copy the Transit configuration file to the run directory:

```
cp ../transit/transit/examples/demo/transit_demo.cfg .
```

Run Transit to calculate the spectrum:

```
../transit/transit/transit -c transit_demo.cfg
```


To check out the results, run this Python script:

```
import sys
sys.path.append("../transit/scripts/")
import readtransit as rt
wlength, flux = rt.readspectrum("CH4_demo_spectrum.dat.—Flux", 0)

plt.figure(0, (8,5))
plt.clf()
plt.title("Methane Emission Spectrum")
plt.plot(wlength, flux, "b")
plt.xlabel("Wavelength (um)")
plt.ylabel("Flux (erg s-1 cm-1)")
```

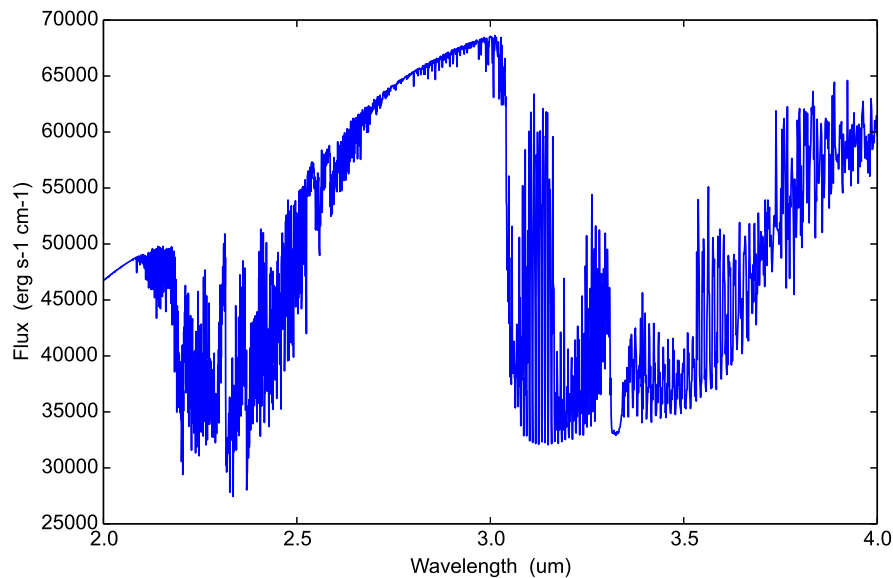


Figure 1: Methane emission spectra.

5 Program Inputs

This Section describes the command-line arguments and input files required by the the `Pylineread` and `Transit` modules, and any additional information needed to properly configure the modules.

5.1 Pylineread

The executable `transit/pylineread/src/pylineread.py` is the main `Pylineread` routine. `Pylineread` runs from the shell taking a set of command-line arguments. Alternatively, the

command-line arguments can be specified using a configuration file. Before running `Pylineread`, the user needs to obtain two types of input files: opacity line-list database files and partition-function files.

5.1.1 Pylineread Command-Line Arguments

To display the complete list of command-line arguments, cd into the `Pylineread` source folder (`transit/pylineread/src`) and execute:

```
./pylineread.py --help
```

Optional Arguments:

- `-h, --help`
Show the help message and exit.
- `-c FILE, --config_file FILE`
Configuration filename (string).
- `-v VERB, --verbose-level VERB`
Verbosity level (Integer) [default: 2].
- `-q, --quiet`
Set verbosity level to 0.

Database Arguments:

- `-o OUTPUT, --output OUTPUT`
Output TLI filename (string) [default: 'output.tli'].
- `-d DB_LIST, --database DB_LIST`
Path (string) to the input line-transition database file(s).
- `-p PART_LIST, --partition PART_LIST`
Path (string) to the auxiliary partition-function file(s).
- `-t DBTYPE, --dbtype DBTYPE`
Database type (string). 'ps' for Partridge & Schwenke's H₂O; 'hit' for HITRAN and HITEMP; or 'ts' for Schwenke's TiO.

Wavelength Arguments:

- `-i IWAV, --wav-init IWAV`
Initial wavelength (microns) [default: 1.0].
- `-f FWAV, --wav-final FWAV`
Final wavelength (microns) [default: 2.0].

5.1.2 Configuration File

A configuration file presents an alternative to the command-line arguments to specify the input variables. The examples folder (`transit/pylineread/examples/`) provides a configuration-

file sample, `pyline_example.cfg`, and is further explained below:

```
[Parameters]
# Multiple-value arguments can be set separated either by a white space or
# a line break.

# This is the list (and source) of the currently supported Line Lists:
# Partridge and Schwenke (H2O):
#   - http://kurucz.harvard.edu/molecules/h2o/h2ofastfix.bin
# HITRAN and HITEMP:
#   - http://www.cfa.harvard.edu/hitran/
# Schwenke (TiO):
#   - http://kurucz.harvard.edu/molecules/tio/tioschwenke.bin

# With the corresponding partition functions:
#   - http://kurucz.harvard.edu/molecules/h2o/h2opartfn.dat
#   - Total Internal Partition Sums (TIPS) *
#   - http://kurucz.harvard.edu/molecules/tio/tiopart.dat
# (*): Transit incorporates a modified version of the TIPS code

# Path(s) to the database line lists:
# (assuming that the user put the files in a databases folder)
db_list = ../databases/Schwenke-H2O/h2ofastfix.bin
        ../databases/HITEMP/CO2/02_2500-3000_HITEMP2010.par

# Path(s) to the partition function files:
part_list= ../databases/Schwenke-H2O/h2opartfn.dat
           ../transit/pylineread/src/fortran/lib/TIPS.BART

# Type of each input database:
#   hit:  HITRAN and HITEMP
#   ps:   Partridge and Schwenke H2O
#   ts:   Schwenke TiO
dbtype   = ps hit

# The output filename
output   = PSandHIT.2.0-4.0um.tli

# Initial wavelength in microns:
iwav     = 2.0

# Final wavelength in microns:
fwav     = 4.0
```

```
# Verbosity level (max number 20)
verb      = 10
```

Pylineread’s configuration files follow the [ConfigParser](#)⁶ format. The [Parameters] line defines the section read by ConfigParser. Multiple arguments can be separated either with blank spaces or put in separated lines. The db_list, part_list, and dbtype arguments must have the same number of values, and should be input in the corresponding order. We recommend that the output name carry a .tli extension.

5.1.3 Opacity Line-List Files

Table 1 lists the line-transition databases that are currently supported by pylineread and source URLs so the user can obtain such files.

Table 1: Line-Transition Databases for Pylineread		
Database	Molecule	URL
Partridge & Schwenke	H ₂ O	kurucz.harvard.edu/molecules/h2o/h2ofastfix.bin
HITRAN	H ₂ O, CO ₂ , CH ₄ , + others	cfa.harvard.edu/hitran
HITEMP	H ₂ O, CO ₂ , CO	cfa.harvard.edu/hitran
Schwenke	TiO	kurucz.harvard.edu/molecules/tio/tioschwenke.bin

5.1.4 Partition-Function Files

Table 2 lists the partition-function files and source URLs for the databases listed in Table 1. For the HITRAN and HITEMP databases, Pylineread provides a modified version of the Total Internal Partition Sums (TIPS, Laraia et al., [2011](#)) code⁷, to calculate the partition functions.

Table 2: Partition-Function Data for Pylineread		
Database	Temperature range (K)	URL
Partridge & Schwenke	10-6000	kurucz.harvard.edu/molecules/h2o/h2opartfn.dat
HITRAN & HITEMP	70-3000	transit/pylineread/src/fortran/lib/TIPS_BART
Schwenke	10-6000	kurucz.harvard.edu/molecules/tio/tiopart.dat

5.1.5 HITRAN Data File

The HITRAN data file, `transit/pylineread/inputs/hitran.dat`, is an additional file used by Pylineread to obtain known physical properties of the species from the HITRAN and HITEMP databases. This file is automatically read by Pylineread and, thus, does not need to be given as

⁶docs.python.org/2/library/configparser.html

⁷faculty.uml.edu/robert_gamache/software/index.htm

an argument. There is also no need to modify this file by the user, as the information included does not vary. The layout of the `hitran.dat` is given below:

```
# ID:           HITRAN molecule ID
# Molecule:    Molecule name
# Iso:          Isotope AFGL code
# gi:           State-independent Statistical weight
# Iso ratio:    Isotopic ratio
# Iso mass:     Isotopic mass (amu)
```

#	ID	Molecule	Iso	gi	Iso ratio	Iso mass
1	H2O	161	1	9.973e-01	18.0105646	
1	H2O	181	1	1.999e-03	20.014811	
1	H2O	171	6	3.719e-04	19.014781	
1	H2O	162	6	3.107e-04	19.016841	
1	H2O	182	6	6.230e-07	21.021088	
1	H2O	172	36	1.158e-07	20.021058	
2	CO2	626	1	9.842e-01	43.98982920	
2	CO2	636	2	1.106e-02	44.99318400	
...	

The first, second, and third columns are the molecular ID, molecule names, and isotope ID, respectively, as given by the HITRAN database. The fourth column (g_i) are the state-independent statistical weights (from Fischer et al., 2003), the fifth column are the isotopic ratios (from Šimečková et al., 2006), and the last column are the isotopic masses (calculated from Lide, 2008).

5.2 Transit

The executable `transit/transit/transit` is the main Transit routine. Transit runs from the shell taking a set of command-line arguments. Alternatively, the command-line arguments can be specified using a configuration file. Before running Transit, the user needs to obtain three types of input files, an atmospheric file, transit-line information (TLI) files (created by Pylineread), and collision-induced absorption (CIA) files. Additionally, Transit uses a molecules data file (included in the code). Lastly, an optional opacity file can be used to provide a pre-calculated table of opacities (this file can be created by Transit itself).

5.2.1 Transit Command-Line Arguments

To display the complete list of command-line arguments, `cd` into the Transit source folder (`transit/transit`) and execute:

```
./transit --help
```

General Options:

```
-h, --help
```

Display the list of command-line arguments.

-V, --version

Display Transit's version number.

-q, --quiet

Set the verbosity level to the minimum.

-v, --verb=<verb>

Set the verbosity level (integer) to <verb>. [default: 2].

-c, --config_file=<file>

Read command-line arguments from <file>.

Input/Output Options:

-o, --output=<outfile>

Output file to store the model spectrum. [default: Print to standard output].

--atm=<atmfile>

Input atmospheric info file.

--linedb=<linedb>

Input line information (TLI) file(s) (as given by 'pylineread').

--cia=<filenames>

Input collision-induced absorption (CIA) opacities file(s) (comma-separated list if more than one file).

--outtoomuch=<filename>

Output file to store the depth (as a function of wavelength) where the optical depth reached 'toomuch'.

--outsample=<filename>

Output file to store the layer and wavenumber sampling information. A dash (-) indicates standard input. [Default: NULL].

(FINDME: Standard input?)

--molfile=<filename>

Input file with the molecular information. [default: ../inputs/molecules.dat].

Radius Options:

--raddelt=<spacing>

Radius spacing. If set, resample the atmospheric layers to an equidistant sampling array. [default: -1].

--radlow=<radius>

Lower radius. If 0, use atmospheric-file minimum. [default: 0].

--radhigh=<radius>

Higher radius. If 0, use atmospheric-file maximum. [default: 0].

--radfct=<factor>
Radius units conversion factor to cm. E.g., if the radii are given in m, then radfct=100. If 0, use the atmospheric-file factor. [default: 0].

Atmospheric Options:

--allowq=<value>
Maximum allowed cumulative-abundance departure from 1.0. [default: 0.00001].

--refpress=<value>
Atmospheric pressure at the planet's reference 'surface'.

--refradius=<value>
Atmospheric radius at the planet's reference 'surface'.

--gsurf=<value>
Planetary surface (bulk) gravity (in cm/s²).

--qmol=<NULL>
List of molecule names to modify their abundance with qscale.

--qscale=<NULL>
log10-abundance scale factors for qmol molecules.

Wavelength-Array Options (in wlfct units):

--wllow=<wavel>
Lower wavelength boundary. [default: Minimum in TLI file].

--wlhigh=<wavel>
Upper wavelength boundary. [default: Maximum in TLI file].

--wlfct=<factor>
Wavelength units conversion factor to cm. E.g., for wavelengths given in microns, wlfct=1e-4. [default: 1.0].

Wavenumber-Array Options (in wnfc units):

--wnlow=<waven>
Lower wavenumber boundary. [default: wavelength maximum boundary].

--wnhigh=<waven>
Upper wavenumber boundary. [default: wavelength minimum boundary].

--wndelt=<spacing>
Wavenumber array spacing. [default: 1].

--wnosamp=<Integer>
Wavenumber oversampling factor. [default: $2160 = 2^4 \times 3^3 \times 5$].

--wnfc=<factor>
Wavenumber units conversion factor to cm⁻¹. [default: 1.0].

Voigt Profile Calculation Options:

- ndop=<integer>**
Number of Doppler-broadening width samples [default: 40].
- nlor=<integer>**
Number of Doppler-broadening width samples [default: 40].
- dmin=<float>**
Minimum Doppler-broadening width (in cm-1) [default: 1e-3].
- dmax=<float>**
Maximum Doppler-broadening width (in cm-1) [default: 0.25].
- lmin=<float>**
Minimum Lorentz-broadening width (in cm-1) [default: 1e-4].
- lmax=<float>**
Maximum Lorentz-broadening width (in cm-1) [default: 10.0].
- nwidth=<number>**
Number of the max-widths (the greater of Voigt or Doppler widths) that needs to be contained in a calculated profile. [default: 20].

Extinction-Coefficient Calculation Options:

- ethresh=<threshold>**
Minimum extinction-coefficient ratio (w.r.t. maximum in a given layer) to consider in the calculation. [default: 1e-8].
- cloudrad=<radup, raddown>**
If set (in conjunction with cloudext), define a cloud layer (gray opacity component) where a gray opacity component linearly increases from radup to raddown, where the opacity will reach cloudext. From raddown below keep constant opacity. Use '--cloudfct' units; if not defined, use radfct.
- cloudext=<extinction>**
Maximum extinction of the cloud, which opacity will linearly increase from 'radup' to 'raddown'.
- cloudfct=<factor>**
Radius units conversion factor to cgs for --cloudrad.
- detailext=<filename:wn1,wn2,...>**
Save extinction at specified wavenumbers in filename.
- detailcia=<filename:wn1,wn2,...>**
Save CIA extinction at specified wavenumbers in filename.
- saveext=<filename>**
Save extinction array in this file which won't need to be recomputed if only the radius scale (scale height) changes.

Opacity-Grid Options:

- opacityfile=<filename>
Filename to read/save the opacity grid.
- tlow=<temperature>
Lower temperature boundary for the opacity grid (in kelvin). [default: 500].
- thigh=<temperature>
Upper temperature boundary for the opacity grid [default: 3000].
- tempdelt=<spacing>
Temperature sample spacing (in Kelvin degrees). [default: 100.0].
- justopacity=<boolean>
If set, end execution after the opacity-grid calculation.

Optical-Depth Options:

- s, --solution=<sol_name>
Name of the kind of output solution (eclipse or transit). [default: eclipse].
- toomuch=<optdepth>
Maximum optical depth to calculate (at each wavenumber). [default: 20].
- taulevel=<integer>
Calculate the lightray path with a constant (1) or variable (2) index of refraction. [default: 1].
(FINDME: taulevel=1 is the only working option.)
- modlevel=<integer>
On the modulation calculation, If modlevel=1, do not consider limb darkening, if modlevel=-1 do not consider limb darkening and additionally only returns the modulated radius at which extinction becomes one. (default: 1).
- detailtau=<filename:wn1,wn2,..>
Save optical depth at specified wavenumbers in filename.

Geometry Options:

- starrad=<radius_sun>
Stellar radius in solar radius. (default: 1.125).
- gorbpar=<smaxis,time,incl,ecc,long_node,arg_per>
Orbital parameters. Use the above order. Default: 1, 0, 0, 0, 0, 0.
- gorbparfct=<unitsof:smaxis,time,incl,ecc,long_node,arg_per>
Units conversion factors to the cgs system of the orbital parameters. Same order of g-orbpar.
Default: AU, hours, deg, 1, deg, deg.
- transparent

If selected, the planet will have a maximum optical depth given by `toomuch`, it will never be totally opaque.

`--raygrid=<(null)>`

List of incident angles to calculate the emission intensity spectrum (default: 0 20 40 60 80).

(FINDME: re-word this:)

The next sub section describe how the CLA relate to the radiative transfer aspect/case/problem.

5.2.1.1 Spectrum Wavenumber Sampling

Internally, `transit` samples the spectrum in a equi-spaced wavenumber space, in CGS units. However, the user can specify the spectrum boundaries either in wavenumber or wavelength. The `'wnfct'` and `'wlfct'` arguments allow the user to specify the units of the input wavenumber and wavelength variables, respectively.

`Transit` implements a 'dynamic' wavenumber sampling, adjusting the sampling at each layer to avoid oversampling or undersampling the line Voigt profiles, allowing for an efficient extinction coefficient calculation at all layers (see Figure 2).

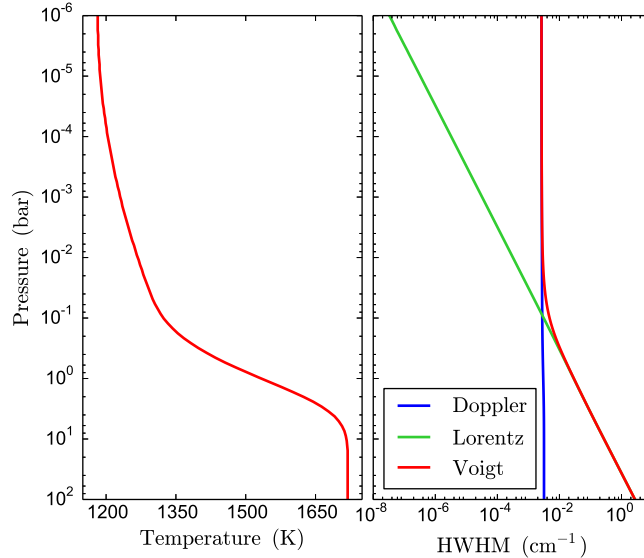


Figure 2: Doppler and Lorentz half-width at half maximum (HWHM) line broadening for the water molecule at 11 μm , for a H_2/He -dominated atmosphere. Since the Lorentz profile width is proportional to the pressure, the Voigt profile HWHM varies over several orders of magnitude between the top and bottom of the atmosphere.

The `'wndelt'` argument defines the 'coarse' sampling interval ($\Delta\nu_c$), which is the sampling of the output spectra. Together with the oversampling-factor argument, `'wnosamp'`, `Transit` defines the 'fine' sampling interval as: $\Delta\nu_f = \text{wndelt} / \text{wnosamp}$. The dynamic sampling interval ($\Delta\nu_d$) lies between the fine and coarse sampling interval.

Initially, `Transit` pre-computes Voigt profiles, for a set of Lorentz and Doppler widths, over the fine sampling. Then, these profiles are decimated to the dynamic sampling to calculate the

extinction coefficient. Lastly, the extinction coefficient is downsampled to the coarse sampling. This requires that the dynamic sampling be an integer factor of the fine sampling ($\Delta\nu_d = f_1\Delta\nu_f$, with $f_1 \in \mathbb{N}$), and the coarse sampling be an integer factor of the dynamical sampling ($\Delta\nu_c = f_2\Delta\nu_d$, with $f_2 \in \mathbb{N}$). Noting that **wnosamp** = f_1f_2 , favorable values of **wnosamp** are thus numbers with a large number of integer divisors.

The ‘**resolv**’ argument (**FINDME: not implement yet**) sets the minimum number of spectral points to sample a profile’s HWHM, determining the dynamic sampling interval for each layer. Given the wavenumber range and the layer’s temperature, pressure, and composition, `Transit` calculates the thinnest HWHM (HWHM_{\min}), then `Transit` selects the largest integer divisor of ‘**wnosamp**’ (d_{\max}) that resolves HWHM_{\min} :

$$\Delta\nu_d = d_{\max} \Delta\nu_f \leq \frac{\text{HWHM}_{\min}}{\text{resolv}}. \quad (1)$$

5.2.1.2 Atmospheric-Layer Sampling

By default, `Transit` uses the atmospheric file’s layer sampling. If the user sets the ‘**raddelt**’ argument, the layers will be resampled to an equi-spaced radius sampling. The radius boundaries can also be redefined with the ‘**radhigh**’ and ‘**radlow**’ arguments.

5.2.1.3 Extinction-Coefficient Calculation

`Transit` has an option to calculate the extinction coefficient on the spot (line-by-line calculation) for each layer, or interpolate from a pre-calculated table of opacities.

By setting the ‘**opacityfile**’ argument, the user chooses to interpolate from the specified opacity table. If the file does not exist, `Transit` will compute (and save) the extinction-coefficient table over a grid of wavenumber, pressure, temperature, and species arrays. The wavenumber is taken from the coarse wavenumber sampling. The pressure array is taken from the atmospheric layers. The list of species will be taken from the TLI file. The temperature array will be computed as a linear sample from ‘**tlow**’ to ‘**thigh**’ with sampling interval ‘**tempdelt**’. If the opacity file exists, `Transit` will check that the table’s wavenumber, pressure, and species list match those specified by the command-line arguments.

Typical runtimes (for a 100-layers atmosphere, 5 million lines, from 3 to 11 μm) to calculate a spectrum with an existing opacity file (interpolation), on the spot (line-by-line calculation), or to generate the opacity file requires a few seconds, minutes, and hours, respectively.

5.2.1.4 Line-by-Line Calculation

The line-by-line calculation of the extinction coefficient (see the theory document) will only consider the contribution from the lines which strength is larger than $S_{\max} \times \text{ethresh}$, with S_{\max} the maximum line-strength in a given layer.

5.2.1.5 Voigt-Profile Calculation

The Voigt profiles used in the line-by-line extinction-coefficient calculation are pre-calculated in a 2D table for a range of Doppler and Lorentz widths. The Doppler range is a log-spaced sample of ‘**ndop**’ widths from ‘**dmin**’ to ‘**dmax**’. Likewise, the Lorentz range is a log-spaced sample of

‘**nlor**’ widths from ‘**lmin**’ to ‘**lmax**’. The ‘**nwidth**’ argument indicates how far from the central wavenumber (in number of profile half-widths) to calculate the Voigt profile.

5.2.1.6 Cloud Opacity

Transit allows for a basic gray-opacity (cloud) layer. The two values of ‘**cloudrad**’ define a the top and bottom radii of a layer where the opacity linearly increasing from zero (at **radup**) up to **cloudext** at **raddown**. Below this level, the opacity remains constant at **cloudext**.

5.2.2 Configuration File

A configuration file presents an alternative to the command-line arguments to specify the input variables. The following example (**transit/run/config.sample.cfg**) shows the format of a basic transit configuration file, which is further explained below:

```
# Transit Configuration File Example:
# Comment (#) and empty lines are allowed.
# To set an argument, write the argument name, followed by the
# argument value (white-space separated). No need for the 'equal'
# sign, nor quotes for string values.
# For the full list of arguments see Transit User Guide or type: transit -h

# ::::::::::: Input files ::::::::::::::::::::::::::::::::::::::::::::
# Path to atmospheric info file:
atm    /home/.../HD209458b_atm.tea
# Path to transit line information (TLI) file:
linedb /home/.../HITRAN_CH4.tli
# Path to collision induced absorption (CIA) file:
cia    /home/.../h2h2.dat

# ::::::::::: Spectrum sampling ::::::::::::::::::::::::::::::::::::::
# Lowest wavelength boundary (also can be set as the wavenumber
# highest boundary with wnhigh):
wllow  2.8
# Highest wavelength boundary (also can be set as the wavenumber
# lowest boundary with wnlow):
wlhigh 11.0
# Conversion factor from wavelength units to cm (default: 1e-4, microns):
wlfct  1e-4
# Wavenumber sampling for plotting the final output (default: 1.0)
wndelt  1.0
# Wavenumber over-sampling factor for internal calculations, see the User Guide
# (default: 2160)
wnosamp 2160
# Conversion factor from wavenumber units to cm-1 (default: 1.0):
```

```

wnfct    1.0

# ::::::::::: Geometry ::::::::::::::::::::::::::::::::::::::::::::
# Eclipse or transit (default: eclipse)
solution eclipse
# Planetary grid for intensity calculation in degrees
#   (default: 0 20 40 60 80)
raygrid 0 20 40 60 80

# ::::::::::: Optical Depth ::::::::::::::::::::::::::::::::::::::::::::
# Maximum optical depth (default: 20)
toomuch 10
# Opacity threshold, see the User Guide (default: 1e-6)
ethresh 1e-6

# ::::::::::: Broadening Function Calculation ::::::::::::::::::::::::::
# Number of HWHM left and right from the Voigt profile centre
#   (default: 20)
nwidth 20

# ::::::::::: Opacity Grid Calculation ::::::::::::::::::::::::::::::::::
# Lowest temperature boundary in K (default: 500)
tlow      500
# Highest temperature boundary in K (default: 3000)
thigh     3000
# Temperature sampling in K (default: 100)
tempdelt  100
# Path to the opacity file
opacityfile ./opacity_CH4.dat

# ::::::::::: Verbosity Level ::::::::::::::::::::::::::::::::::::::::::::
# Level of on-screen verbosity from 1-20 (default: 2)
verb 11

# ::::::::::: Output Files ::::::::::::::::::::::::::::::::::::::::::::
# Wavelength vs. radius where the optical depth reaches toomuch
outtoomuch ./eclipse_toomuch.dat
# Various sampling information
outsample  ./eclipse_sampling.dat
# Final output spectrum, wavelength vs. flux
output     ./eclipse_spectrum.dat

```

Transit's configuration file has its own format. Comment lines start with the # character. When setting an argument-value pair, do not include the 'equal' sign in between. String values do not need the quotation marks.

5.2.3 Atmospheric File

The atmospheric file is a plain text file that determines the species present in the atmosphere and the physical properties of the atmospheric layers (pressure, radius, temperature, and mole mixing ratio of the species) assuming a 1D plane-parallel model. See below (and `transit/examples/example01/sample01.atm`) for an atmospheric file sample: **(FINDME: add file to repo)**

```
# This is a sample atmospheric file for transit.
# HD209458b

# Values units: radius (km), pressure (bar), temperature (K),
#               abundances (unitless).
ur 1e5
up 1e6
q number

#SPECIES
H He C N O H2 CO CO2 CH4 H2O NH3 C2H2 C2H4

#TEADATA
# Radius      Pressure      Temp      H              C              ...      C2H4
 93102.145    1.00000e+02    1887      9.9917414e-01  2.6893119e-04  ...    9.5068e-09
 96092.954    1.7783e+00    1839.85   9.9917414e-01  2.6893119e-04  ...    2.0976e-08
 99008.753    3.1623e-02    1791.37   9.9917414e-01  2.6893119e-04  ...    2.2020e-08
    ...      ...          ...      ...          ...          ...    ...
101851.331    5.6234e-04    1744.45   9.9917414e-01  2.6893119e-04  ...    2.3203e-08
104638.705    1.00000e-05    1701.75   9.9917414e-01  2.6893119e-04  ...    2.4418e-08
```

The atmospheric file follows the following format: Blank and comment lines (starting with the ‘#’ character) are allowed and ignored by transit. The ‘ur’ and ‘up’ keywords set the radius and pressure units (conversion factors to CGS), respectively. For example, if the radii are given in km ($= 10^5$ cm), set ‘ur 1e5’. The ‘q’ keyword indicate if the abundances are given by mass or by number. The line after ‘#SPECIES’ lists the species in the atmosphere. The ‘#TEADATA’ line indicates where the atmospheric data per layer starts. The file contains one layer’s information per line (in descending pressure order). Each line contains the radius, pressure, temperature, and mole mixing ratio for each layer. The file can be produced using the BART routines (see github.com/joe4/BART and documentation therein).

5.2.4 Transit Line Information (TLI) File

The TLI file is a binary file that provides the species’ line-transition information (central wavelength, lower-state energy, and weighted oscillator strength), mass, isotopic ratio, and a tabulated partition-function array as function of temperature for each one. The TLI file is the output of the `Pylineread` module.

5.2.5 CIA File

The CIA file provides tabulated collision-induced absorption data for Transit. CIA data can be obtained from Aleksandra Borysow’s webpage (astro.ku.dk/~aborysow/programs/index.html). See below (and `transit/inputs/CIA_H2H2_400-7000K.dat`) for a CIA file sample:

```
# CIA Header for H2-H2:
i H2 H2
t      1000      2000      3000      4000      5000      6000      7000

# Wavenumber in cm-1, CIA coefficients in cm-1 amagat-2:
 20.00  0.467E-08 0.321E-08 0.283E-08 0.291E-08 0.319E-08 0.351E-08 0.386E-08
 40.00  0.184E-07 0.127E-07 0.113E-07 0.116E-07 0.127E-07 0.140E-07 0.154E-07
 60.00  0.402E-07 0.285E-07 0.253E-07 0.261E-07 0.286E-07 0.315E-07 0.347E-07
    ...
20000.00 0.269E-14 0.567E-12 0.597E-11 0.205E-10 0.382E-10 0.103E-09 0.144E-09
```

A valid CIA file is a plain text file that contains a header and a main body. Comment lines (starting with the ‘#’ character) and blank lines are allowed and ignored by `Transit`. The header must contain two keyword arguments. A line starting with the ‘i’ keyword contains the name of the species separated by blank spaces (names should match those from the atmospheric file). A line starting with the ‘t’ keyword contains the list of temperatures (blank-space separated, in Kelvin degrees) sampled in the CIA file.

The body of the CIA file contains a tabulated list with the absorption coefficients (in units of $\text{cm}^{-1} \text{ amagat}^{-2}$) evaluated as a function of wavenumber (in units of cm^{-1}) and temperature. Each line contains the wavenumber (first column) and the coefficient corresponding to the temperatures specified in the header (values blank-space separated).

5.2.6 Opacity File

The opacity file is a binary file that contains a tabulated grid of extinction coefficients as function of wavenumber, for each species with a line list, and for a range of pressures and temperatures. If specified, `Transit` will use this table to interpolate the extinction coefficient at the temperatures given by the atmospheric profile. The opacity- and atmospheric-file’s pressure arrays must coincide. Likewise, the `transit` and the opacity-file’s wavenumber arrays must also coincide. Similarly, all species in the TLI file must be contained in the opacity file. See Section 5.2.1.3.

5.2.7 Molecules Data File

The molecules data file (`transit/develop/inputs/molecules.dat`) defines a universal ID, the mass, and the (collision) diameter for the species in the atmosphere. The layout of the `molecules.dat` file is given below:

```
# Molecular info:
# Radii sources:
```

```
# 01 http://chem.chem.rochester.edu/~nvd/molecularsieves.html
# 02 Mateucci et al. (2006)
# 03 http://www.webelements.com/compounds (from density and mass calculation)
# 04 Wolfram Alpha + Wikipedia
# 05 http://www.chemspider.com/Molecular-Formula/C2H2
# Mass source: http://www.webqc.org/mmcalt.php
```

# ID	Molecule	Mass	Diameter	Diameter	Long
#	Name	g/mol	Angstrom	source	name
101	H2O	18.01528	3.2	01	Water
102	CH4	16.0425	4.0	01	Methane
103	CO	28.0101	2.8	01	Carbon Monoxide
104	CO2	44.0095	2.8	01	Carbon Dioxide
105	H2	2.01588	2.89	02	Molecular Helium
106	NH3	17.03052	3.6	01	Ammonia
107	TiO	63.8664	3.45	03	Titanium Monoxide
108	VO	66.94090	3.32	03	Vanadium Monoxide
109	O2	31.99880	3.46	02	Molecular Oxygen
110	N2	28.01340	3.64	02	Molecular Nitrogen
111	C2H2	26.0373	5.26	05	Acetylene
112	C2H4	28.0532	5.69	05	Ethylene
113	HCN	27.02534	5.0	05	Hydrogen Cyanide
1	H	1.007940	2.4	01	Hydrogen
2	He	4.0026020	2.0	01	Helium
6	C	12.0107	1.7	04	Carbon
7	N	14.0067	1.55	04	Nitrogen
8	O	15.9994	1.52	04	Oxygen
11	Na	22.98976928	3.72	04	Sodium
19	K	39.09830	4.54	04	Potassium

6 Program Outputs

6.1 Pylineread Output

The output of the `Pylineread` module is a TLI file, described in Section 5.2.4.

6.2 Transit Output

The `Transit` module produces up to five output files: the opacity, the flux spectrum, the intensity spectrum, the sampling information, and the max optical-depth files.

6.2.1 Opacity File

See Section 5.2.6.

6.2.2 Flux Spectrum File

This file contains the calculated modulation (transit geometry) or hemisphere-integrated emission (eclipse geometry) spectrum. The first column shows the wavelength (in μm) and the second column the spectrum (unitless for transit, $\text{erg s}^{-1}\text{cm}^{-1}$ for eclipse). The following example shows this file's layout for an eclipse run:

#wvl [um]	Flux [erg/s/cm]
11	50317.47
10.9879133	44824.9485
10.97585312	41507.0681
...	...
...	...

(FINDME: change -Flux to something more reasonable).

6.2.3 Intensity Spectrum File

This file contains the calculated intensity spectrum at each incident angle (for eclipse geometry). The first column has the wavelength (in μm) and the subsequent columns the planetary emission intensity (in $\text{erg s}^{-1}\text{cm}^{-1}\text{sr}^{-1}$) for each of the angles specified by the 'raygrid' argument. The following example shows the layout of this file:

#wvl [um]	I[0.0 deg]	I[30.0 deg]	I[60.0 deg]	I[80.0 deg]	[erg/s/cm/sr]
11	16020.5901	16020.4135	16019.3219	16016.2266	
10.9879	14731.1128	14682.3188	14512.7771	14116.6959	
...	
...	

6.2.4 Sampling Information File

This file stores the wavenumber, radius, and impact parameter sampling information. Each sampling shows the conversion factor to cgs units, the initial and final sampling values, the spacing interval between samples, the number of elements, the wavenumber sampling's oversample factor, and the radius sampling's list of values for radius. The following example shows the layout of this file:

```
#####  
Wavenumber  Sampling  
  
Factor to cgs units: 1  
Initial value: 909.091  
Final value: 3571.43  
Spacing: 1  
Oversample: 1
```

```

Number of elements: 2663
#####
      Radius      Sampling
-----
Factor to cgs units: 100000
Initial value: 123453
Final value: 140707
Spacing: 100
Number of elements: 173
Values:      123452.85      123552.85
            ...           ...
            ...           ...
#####
      Impact parameter Sampling
-----
Factor to cgs units: 100000
Initial value: 140653
Final value: 123453
Spacing: -100
Oversample: 1
Number of elements: 173
Values:      140652.85      140552.85
            ...           ...
            ...           ...
-----

```

6.2.5 Max Optical-Depth File

This file contains the atmospheric layer's radius where the optical depth reached toomuch, as a function of wavelength. The following example shows the layout of this file:

```

#Wavenumber (cm-1)  Radius at max. calculated depth (cm)
909.0909091         13555285300
910.0909091         13095285300
...                 ...
...                 ...

```

(FINDME: change wavenumber to wavelength)

7 Running Transit

7.1 Running Pylineread

We strongly suggest the use a configuration file to specify the command-line arguments. In that way, the user has a record of the arguments used to create the TLI files. The example provided in

`transit/pylineread/examples/` is further described in Section 5.1.2.

Pylineread can be run from any folder, provided the user gives the path from the working folder to the executable. We recommend to create a folder exclusively to execute Pylineread and hold its results. For example, to run Pylineread from a folder located in `transit/pylineread/TLI/` using a configuration file, `cd` into `transit/pylineread/` and execute from the shell:

```
mkdir TLI
```

```
cd TLI/
```

```
cp ../examples/pyline_example.cfg polyline_run_01.cfg
```

(Edit the configuration file arguments following the format from Section 5.1.2)

```
../src/pylineread.py -c polyline_run_01.cfg
```

7.2 Running Transit

Transit runs in the same way as Pylineread. Thus, the same recommendations from Section 7.1 apply. Although Transit has many command-line arguments, in most cases, most of them can be left as defaults. A minimal example is given in `transit/run/transit_example.cfg`. For example, to run Transit using a configuration file from the `transit/run/` folder, `cd` into that folder and execute from the shell:

```
cp config_sample.cfg transit_run_01.cfg
```

(Edit the configuration file arguments following the format from Section 5.2.2)

```
../transit/transit -c transit_run_01.cfg
```

8 Code Organization

(FINDME: TBD)

8.1 TLI File Format

The data listed in a TLI file, in order as they appear, are listed below:

1. Magic number (endianness)
2. TLI version (short)
3. Line reader version (short)
4. Line reader revision version (short)
5. Initial and final wavelength (doubles)
6. Number of databases (short)
7. For each database:
 - Length (short) and name (string) of the database
 - Length (short) and name (string) of the molecule

- Number of temperature samples (short)
- Number of isotopes (short)
- Temperature array (doubles)
- For each isotope:
 - Length (short) and name (string) of the isotope
 - Mass of the isotope (double)
 - Isotopic ratio (double)
 - Partition function at each temperature (doubles)

8. Line transition information:

- Number of transitions (int)
- Transition's wavelength array (doubles)
- Transition's isotope ID array (shorts)
- Transition's lower-state energy array (doubles)
- Transition's oscillator strength (gf) array (doubles)

8.1.1 Opacity File Format

The opacity file is a binary file that contains a tabulated grid of extinction coefficients as function of wavenumber, for each species with a line list, and for a range of pressures and temperatures.

The data stored in the opacity file are:

- Number of species (integer)
- Number of temperature samples (integer)
- Number of pressure-layer samples (integer)
- Number of wavenumber samples (integer)
- Species ID (array of integers)
- Temperature sample (array of floats)
- Layer's pressure (array of floats)
- Wavenumber array (array of floats)
- Extinction-coefficient (array of floats)

9 Routines

(FINDME: TBD)

9.1 Pylineread Module

(FINDME: TBD)

pylineread routines (transit/pylineread/src/):

[pylineread.py](#):

(FINDME: Explain me). (*)

[driver.py](#):

(FINDME: Explain me).

[db_pands.py](#):

(FINDME: Explain me).

[db_voplez.py](#):

(FINDME: Explain me).

[db_hitran.py](#):

(FINDME: Explain me).

[db_tioschwenke.py](#):

(FINDME: Explain me).

[utils.py](#):

(FINDME: Explain me).

[constants.py](#):

(FINDME: Explain me).

Fortran routines (transit/pylineread/src/fortran/):

[BART_BD_ISO_82_TO_85.for](#):

(FINDME: Explain me).

[BD_ISO_2011.for](#):

(FINDME: Explain me).

[BD_MOL_2011.for](#):

(FINDME: Explain me).

[ISOTOPS.CMN](#):

(FINDME: Explain me).

[MOLEC.CMN](#):

(FINDME: Explain me).

[README_TIPS](#):

(FINDME: Explain me).

[SPECIES_2011.CMN](#):

(FINDME: Explain me).

[TIPS_BART.for](#):

(FINDME: Explain me).

Asterisk (*) indicates files that must be executable.

9.2 Transit Module

(**FINDME: TBD**)

Transit routines (transit/transit/src/, in order of execution):

transit.c:

Main routine that calls the rest of the subroutines.

argum.c:

Read and process the user input parameters.

makesample.c:

Create the spectrum, layer, and temperature arrays.

readatm.c:

Read and process the input atmospheric file.

readlineinfo.c:

Read and process the input TLI (transition-lines information) file.

cia.c:

Read and process the collision-induced-absorption files.

idxrefraction.c:

Calculate the index of refraction of the ray-light path.

opacity.c:

Compute the line-broadening profiles and tabulated grid of opacities.

extinction.c:

Compute the extinction coefficient at a given layer.

tau.c:

Calculate the extinction coefficient at each layer for transit geometry.

slantpath.c:

Calculate the transit ray-path and integrated the extinction to calculate the optical depth.

observable.c:

Integrate the optical depth compute the transit modulation.

eclipse.c:

Compute the extinction coefficient and optical depth. Integrate the optical depth to calculate the planet intensity. Integrate the intensity to obtain the planetary emission spectrum (flux).

transitstd.c:

(**FINDME: Explain me**).

geometry.c:

(**FINDME: Explain me**).

MPItransit.c:

Main transit routine for use with the BART project.

9.3 PU Module

pu routines (/transit/pu/src/):

[iomisc.c](#):

(FINDME: Explain me).

[numerical.c](#):

(FINDME: Explain me).

[procopt.c](#):

(FINDME: Explain me).

[voigt.c](#):

(FINDME: Explain me).

[messagep.c](#):

(FINDME: Explain me).

[sampling.c](#):

(FINDME: Explain me).

[xmalloc.c](#):

(FINDME: Explain me).

10 Be Kind

Please cite these papers if you found this package useful for your research:

- [Cubillos et al. \(2015\)](#) (in preparation).
- [Blecic et al. \(2015\)](#) (in preparation).
- [Harrington et al. \(2015\)](#) (in preparation).

Thanks!

11 Reproducible Research

(FINDME: TBD)

How to comply with reproducible research.

What to do if you do not edit the code. What to do if you edit the code.

12 Further Reading

(FINDME: TBD, do we need this section?)

References

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