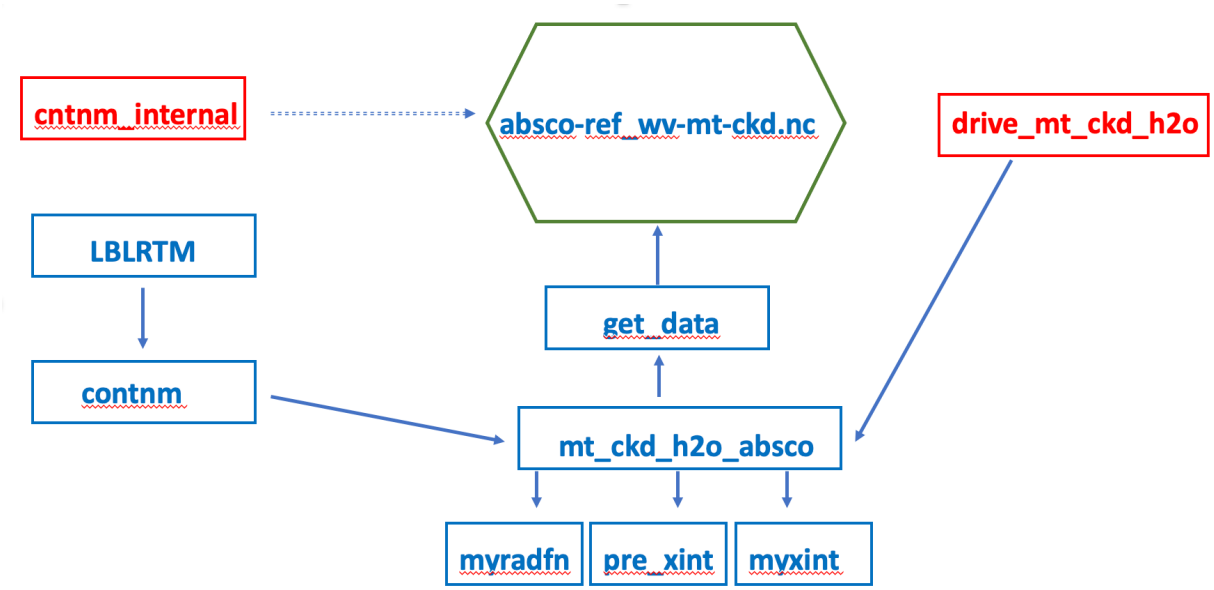
Design for MT-CKD H2O for HITRAN and LBLRTM

1. Flow Chart



2. Components

a. Cntnm_internal: FORTRAN90

This is the internal version of the continuum code, which will allow Eli to continue his continuum development work as he is accustomed to, i.e., modifying the DATA statements and the coefficient calculations. The code outputs the water continuum coefficients in a modern and portable format for use by the mt_ck_h2o routine.

Output: absco-ref_wv-mt-ckd.nc

Below is a listing of the absco-ref_wv-mt-ckd.nc contents:

```
netcdf absco-ref_wv-mt-ckd {
dimensions:
        wavenumbers = 2001 ;
variables:
        double wavenumbers(wavenumbers) ;
                wavenumbers:units = "cm-1" ;
                wavenumbers:description = "Spectral domain of water vapor continuum" ;
```

double self_absco_ref(wavenumbers) ;
self_absco_ref:units = "cm**2/molecule cm-1" ;
self_absco_ref:description = "Water vapor self continuum absorption coefficients" ;
double for_absco_ref(wavenumbers) ;
for_absco_ref:units = "cm**2/molecule cm-1" ;
for_absco_ref:description = "Water vapor foreign continuum absorption coefficients" ;
double self_texp(wavenumbers) ;
self_texp:units = "dimensionless" ;
self_texp:description = "Temperature exponent for water vapor self continuum" ;
double ref_press ;
ref_press:units = "mbar" ;
ref_press:description = "Reference pressure" ;
double ref_temp ;
ref_temp:units = "K" ;
ref_temp:description = "Reference temperature" ;
double ref_h2o_vmr ;
ref_h2o_vmr:units = "vmr" ;
ref_h2o_vmr:description = "Reference H2O Mixing Ratio" ;

// global attributes:
:title = " The MT_CKD Water Vapor Continuum - v4.0 " ;
:copyright = "Copyright ©, Atmospheric and Environmental Research, Inc., 2022 All rights reserved. This source code was developed as part of the LBLRTM software and is designed for scientific and research purposes. Atmospheric and Environmental Research Inc. (AER) grants USER the right to download, install, use and copy this software for scientific and research purposes only. This software may be redistributed as long as this copyright notice is reproduced on any copy made and appropriate acknowledgment is given to AER. This software or any modified version of this software may not be incorporated into proprietary software or commercial software offered for sale without the express written consent of AER. This software is provided as is without any express or implied warranties." ;
:contact = " Address questions to: aer_contnm@aer.com " ;
:reference = " General reference: Mlawer et al. (2012), doi:10.1098/rsta.2011.0295 " ;
:history = "MT_CKD_4.0: water vapor continuum data is now stored in a netCDF file and the code is in a separate module.For previous versions see (http://github.com/AER-RC/MT_CKD). " ;

b. mt_ckd_h2o_module: FORTRAN90

This module contains the mt_ckd_h2o_absco subroutine, which reads in the absco-ref_wv-mt-ckd netCDF file and calculates the water vapor continuum absorption coefficients for the requested pressure, temperature, and spectral range. The mt_ckd_h2o_absco subroutine can

be called from a simple driver (see section d) or from the LBLRTM CONTNM subroutine: it replaces the lines of code, including DATA statements and spectral interpolation, that are currently required in the CONTNM routine for the water vapor continuum absorption calculation. The output is provided in the sh2o and fh2o arrays, which must be declared in the calling program. The module also contains three short private routines adapted from LBLRTM: myradfn, myxint and pre_xint.

mt_ckd_h2o_absco uses the get_data routine in the read_data module to read in absco-ref-wv-mt-ckd.nc file. The module will be provided to SAO, along with the read_data module, the absco-ref_wv-mt-ckd.nc file and a simple FORTRAN driver to run the module.

mt_ckd_h2o_absco

Definition: subroutine mt_ckd_h2o(p_atm,t_atm ,h2o_frac,wv1,wv2,dwv,self_absco, for_absco, radflag)

Inputs:

p_atm - atmospheric pressure for the calculation of continuum coefficients (mbar)
t_atm - atmospheric temperature for the calculation of continuum coefficients (K)
h2o_frac - fraction of the total number of molecules that are water vapor
wv1abs - initial wavenumber for which continuum coefficients will be computed (cm-1)
wv2abs - final wavenumber for which continuum coefficients will be computed (cm-1)
dvabs - wavenumber spacing for the continuum coefficient calculation (cm-1)
radflag - (optional) if true, multiply by radiation term (default); if false, do not

Input/Output:

self_absco - computed water vapor self continuum absorption coefficients (cm2/molecules or 1/(cm-1 molecules/cm2)
for_absco - computed water vapor foreign continuum absorption coefficients (cm2/molecules or 1/(cm-1 molecules/cm2)

myradfn: calculates the radiation term for a specific temperature and an array of frequencies. Note that the radfn function in LBLRTM calculates this term for a single frequency

Definition: integer function myradfn (vi,xkt,nvi,rad)

Inputs:

v1: array of frequencies (cm-1)
xkt: ratio of layer temperature to radcn2 (cm-1)
nvi: number of frequencies in v1

Outputs:

rad: array of radiation terms (cm-1)

pre_xint: finds the starting and ending indices to use in the interpolation to the requested grid

Definition: subroutine pre_xint(v1ss,v2ss,v1abs,dvabs,nptabs,ist,lst)

Inputs:

v1ss:	first frequency of coefficient grid (cm-1)
v2ss:	last frequency of coefficient grid (cm-1)
v1abs:	first frequency of output grid (cm-1)
v2abs:	last frequency of output grid (cm-1)
dvabs:	resolution of output grid (cm-1)
nptabs:	number of points in output grid

Outputs:

ist: index of first point to interpolate to in output grid
lst: index of last point to interpolate to in output grid

myxint: interpolates to output grid and adds to existing absorption/optical depth

Definition: subroutine myxint(v1a,v2a,dva,a,afact,vft,dvr3,r3,n1r3,n2r3)

Inputs:

v1a:	first frequency of coefficient grid (cm-1)
v2a:	last frequency of coefficient grid (cm-1)
dva:	resolution of coefficient grid (cm-1)
a:	array of calculated absorption (cm2/molec) or optical depth
afact:	1.0
vft:	starting frequency of output grid (cm-1)
dvr3:	resolution of output grid (cm-1)
n1r3:	index of first point to interpolate to in output grid
n2r3:	index of last point to interpolate to in output grid

Input/Output

r3: array of interpolated and summed absorption (molec/cm2) or optical depth

c. read_ module: FORTRAN90

This module defines a data type (data2read) to store the contents of absco-ref_wv-mt-ckd.nc, reads in the contents of this file with the get_data routine and returns them to the calling routine in the defined datatype.

Input: absco-ref_wv-mt-ckd.nc

Output: dat: user defined datatype data2read containing all the data in absco-ref_wv-mt-ckd.nc:

```
type data2read
   real(kind=8), allocatable, dimension(:) :: wavenumber
   real(kind=8), allocatable, dimension(:) :: for_absco_ref
   real(kind=8), allocatable, dimension(:) :: self_absco_ref
   real(kind=8), allocatable, dimension(:) :: self_texp
```

d. drive_mt_ckd_h20.f90: FORTRAN

drive_mt_ckd_h2o is a simple FORTRAN driver for mt_ckd_h2o. It reads in the required inputs for absco-ref_mt-ckd-h2o from a NAMELIST file and outputs the spectral grid and the self and foreign coefficients in a netCDF file.

Below is a sample namelist file:

```
&mt_ckd_input
        p_atm=1013.
        t_atm=300.
        h2o_frac= 0.00990098
        wv1=497.
        wv2=603.
        dwv=1.
/
```

The code is compiled with the following command in the build directory (see section **3.**)

```
make -f make_mt_ckd_h2o linuxGNUdbl
```

where make_mt_ckd_h2o is the Makefile and linuxGNUdbl indicates the user has requested the gfortran compiler with double precision.

This command generates the mt_ckd_h2o_v1.0_linux_gnu_dbl executable, which is run as indicated below:

```
mt_ckd_h2o_v1.0_linux_gnu_dbl < mt_ckd.config
```

where mt_ckd.config is the namelist file.

The output is stored in mt_ckd_h2o_output.nc:

```
netcdf mt_ckd_h2o_output {
dimensions:
        nwvn = 107 ;
variables:
        double wavenumbers(nwvn) ;
                wavenumbers:units = "cm-1" ;
                wavenumbers:description = "Wavenumbers\f" ;
        double self_absorption(nwvn) ;
                self_absorption:units = "cm**2/molecule)" ;
                self_absorption:description = "Water vapor continuum self absorption coefficients"
;
        double frgn_absorption(nwvn) ;
                frgn_absorption:units = "cm**2/molecule)" ;
                frgn_absorption:description = "Water vapor foreign continuum absorption
coefficients"  ;
```

Directory structure

mt_ckd_h2o:

```
absco-ref_wv-mt-ckd.nc      build/       mt_ckd.config  mt_ckd_h2o_output.nc    src/
```

mt_ckd_h2o/build:

```
addlibs.inc   make_mt_ckd_h2o*  mt_ckd_h2o_v1.0_linux_gnu_dbl.obj/   read_file.mod
makefile.common*  mt_ckd_h2o.mod    phys_consts.mod
```

mt_ckd_h2o/src:

```
drive_mt_ckd_h2o.f90  mt_ckd_h2o_module.f90  phys_consts.f90  read_module.f90
```