This HTML file was created by the program doc_tsuite.pl, doc_tsuite.txt contains a tab delimited list of the files.

---

agn_blr_albedo.in

measure Rayleigh scattering of Lya

```
title measure Rayleigh scattering of Lya
# model from Korista, K., & Ferland, G. 1998, ApJ, 495, 672
#
# commands controlling continuum =========
agn 6.683 -1.20 -1.20 -0.90
ionization parameter 1.0
#
# commands for density & abundances =========
init file = "ism.ini"
abundances old solar 84
hden 11.0
#
# commands controlling geometry =========
stop total column density = 23.75
#
# other commands for details =========
iterate
#
# commands controlling output =========
normalize to "C 6" 33.7360
print line faint -1
print lines inward
# the normalizing line is not defined on the emergent line stack
print lines emergent off
save overview "agn_blr_albedo.ovr"
save performance "agn_blr_albedo.per"
save continuum last "agn_blr_albedo.con" units kev
save dr "agn_blr_albedo.dr"
save reflected continuum last "agn_blr_albedo.ref"
save emitted continuum last "agn_blr_albedo.emt"
#
# must assert the luminosity since change in this
# line would appear to change the rest of the spectrum
# agn_blr_albedo.in
# class blr
# ======================================
```

This model computes the albedo of a fairly standard BLR cloud. This is the type of model that was presented in the BLR albedo paper by Korista & Ferland, 1998, ApJ 495, 672.

The asserts then check that these continua have the expected brightness.

---

agn_lex00_u0.in

intermediate-ionization x-ray ionized cloud from Lexington 2000

```
title intermediate-ionization x-ray ionized cloud from Lexington 2000
stop column density 16
print line sort wavelength
print lines column linear
normalize to "H 1" 1215.67A
print line faint -1
hden 5
iterate
```

```
phi(h) 15.477 range 7.353 to 735.3
interpolate (-8 -3)
continue (-6 1.)
continue (-2 14.5)
continue (0.4771 12.7)
continue (0.8663 10.6)
continue (3.8663 7.6)
continue (6 1)
continue (9 -3)
element abundance helium -1
element abundance carbon -3.432
element abundance nitrogen -3.959
element abundance oxygen -3.097
element abundance neon -3.959
element abundance magnesium -4.4318
element abundance silicon -4.456
element abundance sulphur -4.7959
element abundance argon -5.4318
element abundance iron -4.398
element lithium off
element beryllium off
element boron off
element fluorine off
element sodium off
element aluminium off
element phosphrous off
element chlorine off
element potasium off
element calcium off
element scandium off
element titanium off
element vanadium off
element chromium off
element manganese off
element cobalt off
element nickel off
element copper off
element zinc off
#
save overview "agn_lex00_u0.ovr"
save performance "agn_lex00_u0.per"
save transmitted continuum "agn_lex00_u0.trn" units keV
#
# agn_lex00_u0.in
```

This is one of the "warm absorber" simulations presented at the Lexington 2000 meeting on nebulae. Pequignot et al. summarized in 2001ASPC..247..533P. It is necessary to also include the command no induced processes to obtain the results presented there. This disables UTA ionization, a process that was not included in the calculations presented in the paper.

---

agn_lex00_u1.in

high-ionization x-ray ionized cloud from Lexington 2000

```
title high-ionization x-ray ionized cloud from Lexington 2000
stop column density 16
print lines column linear
normalize to "H 1" 1215.67A
print line faint -1
hden 5
iterate
phi(h) 16.477 range 7.353 to 735.3
interpolate (-8 -3)
continue (-6 1.)
continue (-2 14.5)
continue (0.4771 12.7)
```

```
continue (0.8663 10.6)
continue (3.8663 7.6)
continue (6 1)
continue (9 -3)
element abundance helium -1
element abundance carbon -3.432
element abundance nitrogen -3.959
element abundance oxygen -3.097
element abundance neon -3.959
element abundance magnesium -4.4318
element abundance silicon -4.456
element abundance sulphur -4.7959
element abundance argon -5.4318
element abundance iron -4.398
element lithium off
element beryllium off
element boron off
element fluorine off
element sodium off
element aluminium off
element phosphrous off
element chlorine off
element potasium off
element calcium off
element scandium off
element titanium off
element vanadium off
element chromium off
element manganese off
element cobalt off
element nickel off
element copper off
element zinc off
save overview "agn_lex00_u1.ovr"
save performance "agn_lex00_u1.per"
save transmitted continuum "agn_lex00_u1.trn" units keV
#
# agn_lex00_u1.in
```

This is one of the "warm absorber" simulations presented at the Lexington 2000 meeting on nebulae. Pequignot et al. summarized in 2001ASPC..247..533P. It is necessary to also include the command no induced processes to obtain the results presented there. This disables UTA ionization, a process that was not included in the calculations presented in the paper.

---

agn_lex00_um1.in

low-ionization x-ray ionized cloud from Lexington 2000

```
title low-ionization x-ray ionized cloud from Lexington 2000
stop column density 16
print lines column linear
print lines sort intensity
normalize to "H 1" 1215.67A
print line faint -2
hden 5
iterate
phi(h) 14.477 range 7.353 to 735.3
interpolate (-8 -3)
continue (-6 1.)
continue (-2 14.5)
continue (0.4771 12.7)
continue (0.8663 10.6)
continue (3.8663 7.6)
continue (6 1)
continue (9 -3)
element abundance helium -1
```

```
element abundance carbon -3.432
element abundance nitrogen -3.959
element abundance oxygen -3.097
element abundance neon -3.959
element abundance magnesium -4.4318
element abundance silicon -4.456
element abundance sulphur -4.7959
element abundance argon -5.4318
element abundance iron -4.398
element lithium off
element beryllium off
element boron off
element fluorine off
element sodium off
element aluminium off
element phosphrous off
element chlorine off
element potasium off
element calcium off
element scandium off
element titanium off
element vanadium off
element chromium off
element manganese off
element cobalt off
element nickel off
element copper off
element zinc off
#
save overview "agn_lex00_um1.ovr"
save performance "agn_lex00_um1.per"
save transmitted continuum "agn_lex00_um1.trn" units keV
#
# agn_lex00_um1.in
```

This is one of the "warm absorber" simulations presented at the Lexington 2000 meeting on nebulae. Pequignot et al. summarized in 2001ASPC..247..533P. It is necessary to also include the command no induced processes to obtain the results presented there. This disables UTA ionization, a process that was not included in the calculations presented in the paper.

---

agn_reflector.in

model of Compton reflector

```
title model of Compton reflector
#
# commands controlling continuum =========
# this is a powerlaw that extends into the x-rays, but by default
# has exponential cutoff in FIR
power law -1. hi=1000000000
# the ionization parameter for this powerlaw
ionization parameter 1.
# add background so that FIR/radio does not have zero flux
background
iterate
#
# commands for density & abundances =========
hden 11
#
# commands controlling geometry =========
stop total column density 24
#
# other commands for details =========
constant temper 5
database h-like element hydrogen levels resolved 10
database h-like element helium levels resolved 10
```

```
#
# commands controlling output =========
print line faint 1
print line inward
#
# this is to produce lines with lots of contrast with the continuum
set save Line Width 100 km/sec
# a fig in part 3 of hazy uses data from this model. the fig shows lines
# with above and below linewidth
# set save line Width c
save performance "agn_reflector.per"
save continuum last "agn_reflector.con" units kev
save continuum reflected last "agn_reflector.alb" units kev
save overview last "agn_reflector.ovr"
save dr last "agn_reflector.dr"
#
# agn_reflector.in
# class blr
# ======================================
#
```

This is a model of the Compton reflector in AGN. It is a constant temperature since models of this region often make that assumption. A plot in Part I of Hazy shows the incident and reflected portions of the continuum. The code will complain that the cloud is Compton thick since it is not really designed to simulate this situation.

---

agn_S_curve_grid.in

temperature across Spitzer thermal stability S curve

```
title temperature across Spitzer thermal stability S curve
#
# commands controlling continuum =========
# this is the generic AGN continuum
table agn
# the ionization parameter will be varied
ionization parameter 0.00 vary
grid from 0 to 3 in 0.25 dex steps sequential
# add background so that FIR/radio does not have zero flux
background
iterate
#
# commands for density & abundances =========
# intended to make sim run as fast as possible
hden 8
init file "ism.ini"
element sulphur off
element chlorine off
element argon off
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# commands controlling output
# this produces a very large number of lines in the output mostly
# because Hbeta is very weak in hot gas. Choose Lya as the normalization
# line to make line list smaller
normalize to "H 1" 1215.67A
print line faint 10 will be varied
# create file with list of grid parameters
save overview "agn_S_curve_grid.ovr" last no hash
save performance "agn_S_curve_grid.per"
save grid "agn_S_curve_grid.grd" last no hash
save species densities "agn_S_curve_grid.sden" "Si+12[10:11]" last no hash
# save average H+ temperature
```

```
save average "agn_S_curve_grid.avr" last no hash
temperature hydrogen 1
end of temperatures
# save heating and cooling
save heating "agn_S_curve_grid.het" last no hash
save cooling "agn_S_curve_grid.col" last no hash
save pressure "agn_S_curve_grid.pre" last no hash
save iron element "agn_S_curve_grid.fe" last no hash
save xspec atable "agn_S_curve_grid.fit"
save neon element "agn_S_curve_grid.ne" last separate
#
#
# agn_S_grid.in
# class BLR
# ======================================
#
```

This computes a series of models that check the temperature through the S curve in the Fields et al. three-phase model of ISM stability.

---

agn_warm_absorber.in

simple warm absorber model

```
title simple warm absorber model
#
# commands controlling continuum =========
table power law
ionization parameter 0
#
# commands for density & abundances =========
hden 6
abundances old solar 84
#
# commands controlling geometry =========
stop column density 22
#
# other commands for details =========
iterate to convergence
#
# commands controlling output =========
print line faint 10
save overview "agn_warm_absorber.ovr"
save performance "agn_warm_absorber.per"
save continuum "agn_warm_absorber.con" last units kev
save continuum "agn_warm_absorber.conA" last units Angstroms
save fine continuum "agn_warm_absorber.finA" last units Angstroms range 7.6A to 15A merge 3
save dr "agn_warm_absorber.dr" last
save lines, optical depth some, "agn_warm_absorber.opt" last
O 3 5006.84A
end of lines
# this will be the default units, like the printout
save line optical depths last "agn_warm_absorber_lab.lin"
# this will be the same, in rygbergs
save line optical depths last "agn_warm_absorber_ryg.lin" units rydberg
#
# warrm_absorber
# class nlr
# ======================================
#
```

this is a simple warm absorber model. It makes a plot of the transmitted continuum, and generates a list of lines with significant optical depths

---

agn_warm_absorber_hiU.in

simple warm absorber model

```
title simple warm absorber model
set save prefix "agn_warm_absorber_hiU"
#
# commands controlling continuum =========
table power law
ionization parameter 150 linear
#
# commands for density & abundances =========
hden 6
abundances old solar 84
#
# commands controlling geometry =========
stop column density 22
#
# commands controlling models =========
database h-like element zinc collapsed levels 5
#
# other commands for details =========
iterate to convergence
#
# commands controlling output =========
print line column
normalize "Blnd" 1.77982A
save overview ".ovr"
save performance ".per"
save continuum ".con" last units kev
save continuum ".conA" last units Angstroms
save fine continuum ".finA" last units Angstroms range 7.6A to 15A merge 3
save dr ".dr" last
# this will be the default units, like the printout
save line optical depths last ".linkev" unit kev
# this will be the same, in angstrom
save line optical depths last ".lina" -3 units angstrom
#
# warrm_absorber
# class nlr
# ======================================
#
```

This is simple warm absorber model with a high ionization parameter, chosen to yield about 50% ionization fractions for H-like Fe and Zn. It generates a list of lines with significant optical depths.

---

agn_warm_hiu.in

high ionization warm absorber model to test XRISM simulations

```
title high ionization warm absorber model to test XRISM simulations
set save prefix "agn_warm_hiu"
init "XRISM.ini"
iterate to converge
normalize to "Blnd" 1.77982A
#save xspec mtable ".fits"
#save xspec atable ".fits"
#save xspec atable incident continuum ".fits"
#save xspec atable diffuse continuum ".fits"
power law, slope=-0.8 hi cut 1000 Ryd low cut 10 Ryd
xi 4.0 log
hden 9.0 log power -2
```

```
stop column density 24.0 log
turbulence 100 km/s
print line optical depths
print line column
print line sort wavelength
print line faint -1.
# this will enable the largest possible number of higher ionization Fe lines
database chianti levels max
#
save overview ".ovr" last
save performance ".per"
save element iron ionization ".fe"
save overview ".ovr" last no hash separate
#
# these are affected by RAD 2020ApJ...901...68C
# Fe 25 w 1.8504 A
# Fe 25 X 1.8554 A
# Fe 25 y 1.8595 A
# Fe 25 z 1.8682 A
# doublet ratio affected by line optical depths 2025A&A...694L..13G
# Fe 26 1.77802A
# Fe 26 1.78337A
```

#This and the following commands are ignored because of the empty line. #This part of the file can be used for comments or notes. #save line list absolute ".lin" last no hash "linelist_fe.dat" #save physical condition ".phys" last no hash separate #save continuum ".con" last no hash separate # #save line list absolute "_lines_Fe25.dat" "Lines_Fe25.txt" last no hash units Angstroms #save line list absolute "_lines_Fe26.dat" "Lines_Fe26.txt" last no hash units Angstroms # #save line population "_Fe25.pop" "Lines_Fe25.txt" no hash last separate #save line population "_Fe26.pop" "Lines_Fe26.txt" no hash last separate # save element iron ionization "_Fe.ion" no hash last separate # save lines, optical some, "_Fe26-19.opt" last no hash units Angstroms separate Fe26 1.77802A Fe26 1.78344A Fe26 1.50235A Fe26 1.50350A Fe26 1.42490A Fe26 1.42534A Fe25 1.85040A Fe25 1.85540A Fe25 1.85951A Fe25 1.86819A Fe25 1.57317A Fe25 1.49460A end of lines

---

aperture_beam_int.in

test aperture beam command with intensity

```
title test aperture beam command with intensity
#
# commands for density & abundances =========
hden 0
init file "honly.ini"
#
# other commands for details =========
constant temper 4
#
# commands controlling continuum =========
laser 2
ionization -2
#
# commands controlling geometry =========
stop thickness 10
sphere
aperture beam
#
# commands controlling output =========
save overview "aperture_beam_int.ovr"
save performance "aperture_beam_int.per"
#
# aperture_beam_int.in
# class geometry
# ========================================
```

This is a homogeneous sphere that is especially simple. The model is a test of the aperture command, a command that simulates observing part of an extended object. In this case the aperture is a beam contered on the center of the nebula, with

a line of sight extending through the object.

The code carries along a dummy emission line ("Unit 1") with a constant intensity of 1e-10 erg cm-3 s-1. The line goes through all of the code's infrastructure, and when the calculation is complete, the program confirms that the "luminosity" of the line is the emitting volume times 1e-10. The aperture command is verified by asserting that the emission line has the correct "luminosity". In this case the inner radius is not specified so the returned value is unity.

---

aperture_beam_lum.in

test aperture beam command with luminosity

```
title test aperture beam command with luminosity
#
# commands controlling continuum =========
laser 2
q(h) 31.5
#
# commands for density & abundances =========
hden 0
init file "honly.ini"
#
# commands controlling geometry =========
stop thickness 1e10 linear cm
radius 9
sphere
aperture beam
#
# other commands for details =========
constant temper 4
#
# commands controlling output =========
save overview "aperture_beam_lum.ovr"
save performance "aperture_beam_lum.per"
#
# aperture_beam_lum.in
# class geometry
# ======================================
```

This is a homogeneous sphere that is especially simple. The model is a test of the aperture command, a command that simulates observing part of an extended object. In this case the aperture is a beam contered on the center of the nebula, with a line of sight extending through the object.

The code carries along a dummy emission line ("Unit 1") with a constant intensity of 1e-10 erg cm-3 s-1. The line goes through all of the code's infrastructure, and when the calculation is complete, the program confirms that the "luminosity" of the line is the emitting volume times 1e-10. The aperture command is verified by asserting that this emission line has the correct "luminosity".

---

aperture_slit.in

test aperture slit command with luminosity

```
title test aperture slit command with luminosity
#
# commands controlling continuum =========
laser 2
q(h) 31.5
#
# commands for density & abundances =========
hden 0
```

```
init file "honly.ini"
#
# commands controlling geometry =========
radius 9 10
sphere
aperture slit
#
# other commands for details =========
constant temper 4
#
# commands controlling output =========
save overview "aperture_slit.ovr"
save performance "aperture_slit.per"
#
# aperture_slit.in
# class geometry
# ======================================
#
```

This is a homogeneous sphere that is especially simple. The model is a test of the aperture command, a command that simulates observing part of an extended object. In this case the aperture is a long slit contered on the center of the nebula, extending beyond the outer reaches of the matter.

The code carries along a dummy emission line ("Unit 1") with a constant intensity of 1e-10 erg cm-3 s-1. The line goes through all of the code's infrastructure, and when the calculation is complete, the program confirms that the "luminosity" of the line is the emitting volume times 1e-10. The aperture command is verified by asserting that the emission line has the correct "luminosity".

---

blr_f92.in

standard blr cloud in Ferland et al. 1992

```
title standard blr cloud in Ferland et al. 1992
#
# commands controlling continuum =========
table agn
ionization parameter -1
#
# commands for density & abundances =========
hden 11
abundances old solar 84
#
# commands controlling geometry =========
stop column density 25
#
# other commands for details =========
database h-like element hydrogen levels resolved 10
database h-like element helium levels resolved 10
iterate to convergence
#
# commands controlling output =========
print h-like departure hydrogen
print h-like populations hydrogen
print h-like departure helium
print h-like populations helium
normalize to "H 1" 1215.67A = 105.90
print line faint -2
save performance "blr_f92.per"
save overview last "blr_f92.ovr"
save convergence reason "blr_f92.cvr"
save element nitrogen last "blr_f92.nit"
save element calcium last "blr_f92.ca"
save dr "blr_f92.dr"
save transmitted continuum "blr_f92.trn" last
```

```
#
# blr_f92.ini
# class blr
# ======================================
```

This is similar to one of the BLR models presented in Ferland et al. (1992) for the well-studied Seyfert galaxy NGC 5548. It has a very large column density and is marginally optically thick to electron scattering. The spectrum is given relative to Lya, and the intensity of this line is reset to produce a spectrum that is on the same intensity scale as that paper.

---

blr_fp89.in

final F+P 1989 BLR model table 3

```
title final F+P 1989 BLR model table 3
#
# commands controlling continuum =========
table agn
ionization parameter -0.5
#
# commands for density & abundances =========
hden 9.5
init file="c84.ini"
abundances old solar 84
#
# commands controlling geometry =========
stop column density 25.5
#
# other commands for details =========
iterate to convergence
#
# commands controlling output =========
# set a relatively high faint level since lines relative to Lya=100
print line faint -1
print h-like departure coefficients hydrogen
normalize to "H 1" 1215.67A = 85.60
save performance "blr_fp89.per"
save heating "blr_fp89.het"
save convergence reason "blr_fp89.cvr"
save cooling "blr_fp89.col"
save overview last "blr_fp89.ovr"
save element nitrogen last "blr_fp89.nit"
save results last "blr_fp89.rlt"
save dr "blr_fp89.dr"
#
# blr_fp89.in
# class blr
# ======================================
```

Ferland and Persson (1989) presented this calculation of a BLR cloud. The differences between the present predictions and those given by FP are largely due to improved treatment of Balmer line escape and destruction. The spectrum is given relative to a Lya intensity of 100. The column density is VERY large, to reproduce intensities of low-ionization lines, especially the Ca II lines.

---

blr_hizqso.in

high Z quasar cloud

```
title high Z quasar cloud
#
# commands controlling continuum =========
```

```
table agn
ionization parameter 1
#
# commands for density & abundances =========
# actual elec den will be about 100x larger
hden 8
abundances starburst 35
#
# commands controlling geometry =========
# this is more gramage than it appears because of high Z
stop column density 21
#
# other commands for details =========
# once elec den fail occurs due to tripping over He+ - He I-front
# code does recover so not a problem. The default for this is 10,
# and is set low because (hopefully) this would never occur
# hydrogen is a minor constituent in this high metallicity gas
# the electron density is well above the hydrogen density
failures 3
iterate 3
#
# commands controlling output =========
normalize "blnd" 1909
save performance "blr_hizqso.per"
save dr "blr_hizqso.dr"
save convergence reason "blr_hizqso.cvr"
save overview last "blr_hizqso.ovr"
save element nitrogen last "blr_hizqso.nit"
save element chlorine last "blr_hizqso.cl"
save element iron last "blr_hizqso.fe"
save element neon last "blr_hizqso.ne"
save element calcium last "blr_hizqso.ca"
save element zinc last "blr_hizqso.zn"
save heating last "blr_hizqso.het"
save cooling last "blr_hizqso.col"
#
#
# blr_hizqso.in
# class blr
# ======================================
```

This is a model of a very high metallicty BLR cloud. It checks the intensities of some of the brigher lines, and is a check that the code can converge a cloud with this high Z.

Secondary ionization is very important when H is highly ionized, due to very high He abundance. Sec ionization becomes important at the He+ - He ionization front, where H+/H is 1e-5.

---

blr_kk81.in

old blr

```
title old blr
#
# commands controlling continuum =========
interpolate (0 -5) (.05 -5) (.1 0) (1 -0.5) (7.353 -2.233)
continue (735 -3.233) (800 -15) (8.e6 -15)
f(nu) -7.32148
constant gas pressure
#
# commands for density & abundances =========
hden 9.60206
init file="c84.ini"
abundances he=-1 c=-3.699 n=-4 o=-3.1549 ne=-4 na=-8 mg=-4.5229
continue al=-10 si=-4.4229 s=-10 ar=-10 ca=-10 fe=-4.5229 ni=-8
#
```

```
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
failures 2
iterate to convergence
#
# commands controlling output =========
print line faint -1
print ages
normalize "H  1" 1215.67A 100
save performance "blr_kk81.per"
save overview last "blr_kk81.ovr"
save convergence reason last "blr_kk81.cvr"
save dr last "blr_kk81.dr"
save continuum last "blr_kk81.con"
save ionizing continuum "blr_kk81.ion"
#
#
# blr_kk81.in
# class blr
# ======================================
#
```

This is the "standard" BLR model presented by Kwan and Krolik (1981).

>>refer blr cloud Kwan, J., & Krolik, J. 1981, ApJ, 250, 478

Compare line intensities to previous versions of CLOUDY by entering into table on page Error! Bookmark not defined..

The code caution that the resulting total pressure was not constant is to be expected. The KK calculation assumed constant gas pressure, but internally generature line radiation pressure is significant. Because of this the sum of gas plus radiation pressure was not constant although the gas pressure was.

---

blr_level2.in

test dominant level2 lines

```
title test dominant level2 lines
#
# commands controlling continuum =========
table agn
ionization -2
#
# commands controlling geometry =========
stop column density 19
#
# commands for density & abundances =========
hden 10
element phosphorus abundance 0
#
# other commands for details =========
iterate
#
# commands controlling output =========
save performance "blr_level2.per"
save convergence reason last "blr_level2.cvr"
save overview "blr_level2.ovr"
save dr "blr_level2.dr"
#
# blr_level2.in
# class blr
# ======================================
```

This model checks predictions for the "level2" lines. These are lines that are normally very weak, have Opacity Project wavelengths, and g-bar collision strengths. Phosphorus is given a large abundance so that its level2 lines are significant.

---

blr_n09_p18.in

BLR model, density 1e09 cm-3, flux of H-ion phots 1e18 cm2 s-1

```
title BLR model, density 1e09 cm-3, flux of H-ion phots 1e18 cm2 s-1
#
# commands controlling continuum =========
table agn
phi(h) 18
#
# commands for density & abundances =========
hden 9
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
init "c84.ini"
iterate convergence
# these are to try to speed things up
no level2 lines
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
save performance "blr_n09_p18.per"
save overview "blr_n09_p18.ovr" last
save dr "blr_n09_p18.dr" last
save convergence reason "blr_n09_p18.cvr"
#
# blr_n09_p18.in
# class blr
# ======================================
```

This is one of the 5 models that sample the LOC plane.

---

blr_n09_p18_Z20.in

BLR model, density 1e09 cm-3, flux of H-ion phots 1e18 cm2 s-1, Z=20

```
title BLR model, density 1e09 cm-3, flux of H-ion phots 1e18 cm2 s-1, Z=20
#
# commands controlling continuum =========
table agn
phi(h) 18
#
# commands for density & abundances =========
hden 9
abundances starburst 20
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
iterate to convergence
# these are to try to speed things up
init "c84.ini"
no level2 lines
#
```

```
# commands controlling output =========
normalize to "H 1" 1215.67A 100
print h-like hydrogen departure coefficients
save performance "blr_n09_p18_Z20.per"
save overview "blr_n09_p18_Z20.ovr"
save dr "blr_n09_p18_Z20.dr"
save convergence reason "blr_n09_p18_Z20.cvr"
save convergence error "blr_n09_p18_Z20.cve"
#
# blr_n09_p18_Z20.in
# class blr
# ======================================
```

This is one of the 5 models that sample the LOC plane.

---

blr_n09_p20.in

BLR model, density 1e09 cm-3, flux of H-ion phots 1e20 cm2 s-1

```
title BLR model, density 1e09 cm-3, flux of H-ion phots 1e20 cm2 s-1
#
# commands controlling continuum =========
table agn
phi(h) 20
#
# commands for density & abundances =========
hden 9
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
init "c84.ini"
iterate convergence
# these are to try to speed things up
no level2 lines
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
save performance "blr_n09_p20.per"
save overview "blr_n09_p20.ovr" last
save dr "blr_n09_p20.dr" last
save continuum units Angstroms "blr_n09_p20.con" last
save convergence reason "blr_n09_p20.cvr"
#
# blr_n09_p18.in
# class blr
# ======================================
```

This is one of the 5 models that sample the LOC plane.

---

blr_n09_p20_Z20.in

BLR model, density 1e09 cm-3, flux of H-ion phots 1e20 cm2 s-1, Z=20

```
title BLR model, density 1e09 cm-3, flux of H-ion phots 1e20 cm2 s-1, Z=20
#
# commands controlling continuum =========
table agn
phi(h) 20
#
```

```
# commands for density & abundances =========
abundances starburst 20
hden 9
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
init "c84.ini"
iterate convergence
# these are to try to speed things up
no level2 lines
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
save performance "blr_n09_p20_Z20.per"
save overview "blr_n09_p20_Z20.ovr" last
save dr "blr_n09_p20_Z20.dr" last
save convergence reason "blr_n09_p20_Z20.cvr"
#
# blr_n09_p20_Z20.in
# class blr
# ======================================
```

This is one of the 5 models that sample the LOC plane.

This simulation is optically thin in the Lyman continuum - no H ionization front is present. As a result it can be difficult to converge.

---

blr_n09_p22.in

BLR model, density 1e09 cm-3, flux of H-ion phots 1e20 cm2 s-1

```
title BLR model, density 1e09 cm-3, flux of H-ion phots 1e20 cm2 s-1
#
# commands controlling continuum =========
table agn
phi(h) 22
#
# commands for density & abundances =========
hden 9
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
init "c84.ini"
iterate convergence
# these are to try to speed things up
no level2 lines
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
save performance "blr_n09_p22.per"
save overview "blr_n09_p22.ovr" last
save dr "blr_n09_p22.dr" last
save convergence reason "blr_n09_p22.cvr"
#
# blr_n09_p22.in
# class blr
# ======================================
```

This is one of the models that sample the LOC plane.

---

blr_n09_p22_Z20.in

BLR model, density 1e09 cm-3, flux of H-ion phots 1e22 cm2 s-1, Z=20

```
title BLR model, density 1e09 cm-3, flux of H-ion phots 1e22 cm2 s-1, Z=20
#
# commands controlling continuum =========
table agn
phi(h) 22
#
# commands for density & abundances =========
abundances starburst 20
hden 9
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
init "c84.ini"
iterate convergence
# these are to try to speed things up
no level2 lines
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
save performance "blr_n09_p22_Z20.per"
save overview "blr_n09_p22_Z20.ovr" last
save dr "blr_n09_p22_Z20.dr" last
save convergence reason "blr_n09_p22_Z20.cvr"
save convergence base "blr_n09_p22_Z20.cvb"
save element iron "blr_n09_p22_Z20.fe"
# save line emissivities when there is significant ionization stratification
# some of these ions will not exist at the inner edge or even anywhere in the sim
# saving the emissivities should still work correctly though...
save line emissivity "blr_n09_p22_Z20.ems"
Fe21 142.281A
blnd 1666A
O 1 6300.30
He 1 6678.15A
blnd 1240A
end of lines
#
# blr_n09_p22_Z20.in
# class blr
# ======================================
```

This is one of the models that sample the LOC plane.

---

blr_n11_p20.in

BLR model, density 1e11 cm-3, flux of H-ion phots 1e20 cm2 s-1

```
title BLR model, density 1e11 cm-3, flux of H-ion phots 1e20 cm2 s-1
#
# commands controlling continuum =========
table agn
phi(h) 20
#
# commands for density & abundances =========
hden 11
#
# commands controlling geometry =========
stop column density 23
```

```
#
# other commands for details =========
iterate convergence
# these are to try to speed things up
init "c84.ini"
no level2 lines
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
save performance "blr_n11_p20.per"
save convergence reason "blr_n11_p20.cvr"
save overview "blr_n11_p20.ovr" last
save dr "blr_n11_p20.dr" last
#
# blr_n11_p20.in
# class blr
# ======================================
#
```

This is one of the 5 models that sample the LOC plane.

---

blr_n11_p20_Z20.in

BLR model, density 1e11 cm-3, flux of H-ion phots 1e20 cm2 s-1, Z=20

```
title BLR model, density 1e11 cm-3, flux of H-ion phots 1e20 cm2 s-1, Z=20
#
# commands controlling continuum =========
table agn
phi(h) 20
#
# commands for density & abundances =========
hden 11
abundances starburst 20
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
iterate convergence
# these are to try to speed things up
init "c84.ini"
no level2 lines
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
save performance "blr_n11_p20_Z20.per"
save cooling "blr_n11_p20_Z20.col"
save convergence reason last "blr_n11_p20_Z20.cvr"
save heating "blr_n11_p20_Z20.het"
save element calcium "blr_n11_p20_Z20.cal"
save overview "blr_n11_p20_Z20.ovr"
save dr "blr_n11_p20_Z20.dr"
save temperature history "blr_n11_p20_Z20.tem"
#
# blr_n11_p20_Z20.in
# class blr
# ======================================
```

This is one of the 5 models that sample the LOC plane.

2010 dec 25 This sim obtains different results for Hb and Fe II with gcc and icc. This is because the sim is not fully converged. Robin's & Peter's notes follow. This will probably be trac ticket #191

results changed with trivial changes in the source - Peter's example follows; This is due to lack of convergence rather than a fundamental difference in physics r4426:

Fe 2 2400A 6.854 1.9161 Fe 2 6200A 6.827 1.8005 Fe 2 2500A 6.984 2.5834 Fe 2 2300A 7.101 3.3854 Fe 2 8900A 6.714 1.3899

r4427:

Fe 2 2400A 6.852 1.9092 Fe 2 6200A 6.923 2.2472 Fe 2 2500A 6.943 2.3504 Fe 2 2300A 7.161 3.8897 Fe 2 8900A 6.671 1.2574

Robin; OK, I ran for 10 iterations with an old vs. new test on the cooling -- no substantial differences were reported.

The ne does seem to wander around quite a bit deep in the model, rather than smoothly converge -- attached plot is for the last iterations 5 to 10 (i.e. from when the code declares convergence in the standard blr_... run onwards). Not so bad as the difference plot which Peter shows, but not great. The temperature convergence seems better.

Suggests to me this may be a problem with poor convergence criteria/hysteresis, with the collisional cooling change just being the butterfly.

there's also an unresolved drop in both ne and H+ around 8.5e11 cm in the first iteration, which might be worth trying to understand.

Peter: It looks like there is a small thermal front in this model near the outer edge, though I derive this only from eyeballing the Te plot. They are quite common in blr models. It would also be a partial explanation of the jerky behavior of the code: gas near such a front will be quite sensitive to changes in cooling and/or heating since the curves are nearly parallel. It is however still worthwhile asking whether we are exacerbating the problem by writing the cooling terms in atom_leveln() the way we do.

Robin: Yes, there is a temperature front exactly at the rear of the slab (it only appears in the later iterations).

email exhange on this was around 2010 dec 22 - 24

---

blr_n12_p19.in

BLR model, density 1e12 cm-3, flux of H-ion phots 1e19 cm2 s-1

```
title BLR model, density 1e12 cm-3, flux of H-ion phots 1e19 cm2 s-1
#
# commands for density & abundances =========
#
# commands controlling continuum =========
table agn
phi(h) 19
#
# commands controlling geometry =========
hden 12
stop column density 23
#
# other commands for details =========
iterate convergence
# these are to try to speed things up
init "c84.ini"
no level2 lines
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
save performance "blr_n12_p19.per"
save convergence reason last "blr_n12_p19.cvr"
save overview "blr_n12_p19.ovr" last
save dr "blr_n12_p19.dr" last
```

```
#
#
# blr_n12_p19.in
# class blr
# ======================================
```

This is one of the 5 models that sample the LOC plane.

---

blr_n12_p19_Z20.in

BLR model, density 1e12 cm-3, flux of H-ion phots 1e19 cm2 s-1, Z=20

```
title BLR model, density 1e12 cm-3, flux of H-ion phots 1e19 cm2 s-1, Z=20
#
# commands controlling continuum =========
table agn
phi(h) 19
#
# commands for density & abundances =========
hden 12
abundances starburst 20
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
failures 5
iterate convergence
# these are to try to speed things up
init "c84.ini"
no level2 lines
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
save performance "blr_n12_p19_Z20.per"
save convergence reason "blr_n12_p19_Z20.cvr"
save overview "blr_n12_p19_Z20.ovr" last
save dr "blr_n12_p19_Z20.dr" last
#
# blr_n12_p19_Z20.in
# class blr
# ======================================
```

This is one of the 5 models that sample the LOC plane.

---

blr_n13_p18.in

BLR model, density 1e13 cm-3, flux of H-ion phots 1e18 cm2 s-1

```
title BLR model, density 1e13 cm-3, flux of H-ion phots 1e18 cm2 s-1
#
# this is a very low ionization cloud
# the conditions, and some lines, are surprisingly sensitive
# to the treatment of hydrogen molecules
#
# commands controlling continuum =========
table agn
phi(h) 18
#
# commands for density & abundances =========
hden 13
```

```
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
iterate to convergence
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
init "c84.ini"
no level2 lines
save performance "blr_n13_p18.per"
save overview "blr_n13_p18.ovr" last
save dr "blr_n13_p18.dr" last
save convergence reason "blr_n13_p18.cvr"
#
# blr_n13_p18.in
# class blr
# ======================================
```

This is one of the 5 models that sample the LOC plane.

---

blr_n13_p18_Z20.in

BLR model, density 1e13 cm-3, flux of H-ion phots 1e18 cm2 s-1, Z=20

```
title BLR model, density 1e13 cm-3, flux of H-ion phots 1e18 cm2 s-1, Z=20
#
# this is a very low ionization cloud
# the conditions, and some lines, are surprisingly sensitive
# to the treatment of hydrogen molecules
# extend stopping temperature to low values to cover full column density
#
# commands controlling continuum =========
phi(h) 18
table agn
#
# commands for density & abundances =========
hden 13
abundances starburst 20
#
# commands controlling geometry =========
stop column density 23
stop temperature 1000
#
# other commands for details =========
# this sim needs roughly 10 iterations to converge
iterate convergence
# these are to try to speed things up
init "c84.ini"
no level2 lines
# abort if too many failures occur - we want to pass this test
# failures 2
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
save performance "blr_n13_p18_Z20.per"
save overview "blr_n13_p18_Z20.ovr" last
save overview "blr_n13_p18_Z20.ovr1"
save dr "blr_n13_p18_Z20.dr" last
save convergence reason "blr_n13_p18_Z20.cvr"
save heating "blr_n13_p18_Z20.het"
save cooling "blr_n13_p18_Z20.col"
#
#
```

```
# blr_n13_p18_Z20.in
# class blr
# ======================================
```

This is one of the 5 models that sample the LOC plane.

---

blr_n13_p22.in

BLR model, density 1e13 cm-3, flux of H-ion phots 1e22 cm2 s-1

```
title BLR model, density 1e13 cm-3, flux of H-ion phots 1e22 cm2 s-1
#
# commands controlling continuum =========
table agn
phi(h) 22
#
# commands for density & abundances =========
hden 13
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
iterate convergence
# these are to try to speed things up
init "c84.ini"
no level2 lines
#
# commands controlling output =========
print h-like departure hydrogen
print h-like departure helium
normalize to "H 1" 1215.67A 100
save performance "blr_n13_p22.per"
save convergence reason last "blr_n13_p22.cvr"
save overview "blr_n13_p22.ovr" last
save dr "blr_n13_p22.dr" last
#
# blr_n13_p22.in
# class blr
# ======================================
```

This is one of the 5 models that sample the LOC plane.

---

blr_n13_p22_Z20.in

BLR model, density 1e13 cm-3, flux of H-ion phots 1e18 cm2 s-1, Z=20

```
title BLR model, density 1e13 cm-3, flux of H-ion phots 1e18 cm2 s-1, Z=20
#
# commands controlling continuum =========
table agn
phi(h) 22
#
# commands for density & abundances =========
hden 13
abundances starburst 20
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
```

```
iterate convergence
# these are to try to speed things up
init "c84.ini"
no level2 lines
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
save performance "blr_n13_p22_Z20.per"
save convergence reason last "blr_n13_p22_Z20.cvr"
save overview "blr_n13_p22_Z20.ovr"
save dr "blr_n13_p22_Z20.dr"
save heating "blr_n13_p22_Z20.het"
save cooling "blr_n13_p22_Z20.col"
#
# blr_n13_p22_Z20.in
# class blr
# ======================================
```

This is one of the 5 models that sample the LOC plane.

---

blr_n14_p18.in

BLR model, density 1e14 cm-3, flux of H-ion phots 1e18 cm2 s-1

```
title BLR model, density 1e14 cm-3, flux of H-ion phots 1e18 cm2 s-1
#
# this is a very low ionization cloud
# the conditions, and some lines, are surprisingly sensitive
# to the treatment of hydrogen molecules
#
# commands controlling continuum =========
table agn
phi(h) 18
#
# commands for density & abundances =========
hden 14
#
# commands controlling geometry =========
stop column density 23
#stop efrac 0.1
#
# other commands for details =========
iterate to convergence
#
# commands controlling output =========
normalize to "H 1" 1215.67A 100
init "c84.ini"
no level2 lines
save performance "blr_n14_p18.per"
save overview "blr_n14_p18.ovr" last
save dr "blr_n14_p18.dr" last
save convergence reason "blr_n14_p18.cvr"
#
# blr_n14_p18.in
# class blr
# ======================================
```

---

blr_n14_p20.in

BLR model, density 1e14 cm-3, flux of H-ion phots 1e20 cm2 s-1

```
title BLR model, density 1e14 cm-3, flux of H-ion phots 1e20 cm2 s-1
#
# commands controlling continuum =========
table agn
phi(h) 20
#
# commands for density & abundances =========
hden 14
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
iterate convergence
# these are to try to speed things up
init "c84.ini"
no level2 lines
#
# commands controlling output =========
print h-like departure hydrogen
print h-like departure helium
normalize to "H 1" 1215.67A 100
save performance "blr_n14_p20.per"
save convergence reason last "blr_n14_p20.cvr"
save overview "blr_n14_p20.ovr" last
save dr "blr_n14_p20.dr" last
#
# blr_n14_p20.in
# class blr
# ======================================
```

---

blr_n14_p22.in

BLR model, density 1e14 cm-3, flux of H-ion phots 1e22 cm2 s-1

```
title BLR model, density 1e14 cm-3, flux of H-ion phots 1e22 cm2 s-1
#
# commands controlling continuum =========
table agn
phi(h) 22
#
# commands for density & abundances =========
hden 14
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
iterate convergence
# these are to try to speed things up
init "c84.ini"
no level2 lines
#
# commands controlling output =========
print h-like departure hydrogen
print h-like departure helium
normalize to "H 1" 1215.67A 100
save performance "blr_n14_p22.per"
save convergence reason last "blr_n14_p22.cvr"
save overview "blr_n14_p22.ovr" last
save dr "blr_n14_p22.dr" last
#
# blr_n14_p22.in
# class blr
# ======================================
```

blr_nf84.in

early model of blr

```
title early model of blr
#
# commands controlling continuum =========
ionization parameter -1.92
power law -1 100 0.01
#
# commands for density & abundances =========
hden 9.5
init, file="ism.ini"
abundances cameron
stop lyman optical 6
#
# commands controlling geometry =========
#
# other commands for details =========
constant gas pressure
iterate to convergence
#
# commands controlling output =========
save performance "blr_nf84.per"
save overview last "blr_nf84.ovr"
save convergence reason last "blr_nf84.cvr"
save dr last "blr_nf84.dr"
save results last "blr_nf84.rlt"
#
# blr_nf84.in
# class blr
# ======================================
#
```

This is an example of a "conventional" BLR calculation. The parameters are similar to those of Table 1 of Netzer and Ferland (1984). Notice that the ratio of Lyalpha to Hbeta ratio is much larger than observed.

>>refer blr model Netzer, H., & Ferland, G. J. 1984, PASP, 96, 593

---

blr_nf84_45deg.in

early model of BLR, with illumination at 45 degree angle

```
title early model of BLR, with illumination at 45 degree angle
#
# commands controlling continuum =========
ionization parameter -1.92
power law -1 100 0.01
# this continuum is a beam coming in at 45 degrees
illumination angle 45 degrees
#
# commands for density & abundances =========
hden 9.5
abundances cameron
stop lyman optical 6
#
# commands controlling geometry =========
#
# other commands for details =========
init file "ism.ini"
constant gas pressure
```

```
iterate to convergence
#
# commands controlling output =========
save performance "blr_nf84_45deg.per"
save overview "blr_nf84_45deg.ovr"
save convergence reason last "blr_nf84_45deg.cvr"
save dr "blr_nf84_45deg.dr"
save results last "blr_nf84_45deg.rlt"
#
# blr_nf84_45deg.in
# class blr
# ======================================
#
```

This is an example of a "conventional" BLR calculation. The parameters are similar to those of Table 1 of Netzer and Ferland (1984). Notice that the ratio of Lyalpha to Hbeta ratio is much larger than observed.

>>refer blr model Netzer, H., & Ferland, G. J. 1984, PASP, 96, 593

---

blr_rnfa.in

table 1 of Rees et al. ApJ 347, 648

```
title table 1 of Rees et al. ApJ 347, 648
#
# commands controlling continuum =========
table agn
ionization parameter -2
#
# commands for density & abundances =========
hden 10
init file="c84.ini"
abundances he= -1 c= -3.328 n= -4.0088 o= -3.0809 ne= -4 na= -20
continue mg= -4.3768 al= -5.5686 si= -4.36653 s= -4.76955
continue ar= -5.4202 ca= -5.6383 fe= -4.4815 ni= -20
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
iterate to convergence
#
# commands controlling output =========
normalize "H 1" 1215.67A = 100
print line faint -1
save performance "blr_rnfa.per"
save overview last "blr_rnfa.ovr"
save convergence reason last "blr_rnfa.cvr"
save continuum last "blr_rnfa.con" units microns
save transmitted continuum last "blr_rnfa.trn" units rydbergs
save element nitrogen last "blr_rnfa.nit"
save dr last "blr_rnfa.dr"
save results last "blr_rnfa.rlt"
#
# blr_rnfa.in
# class blr
# ======================================
#
```

This is the lower density cloud computed in Rees et al. (1989). Table 1 of that paper lists the predictions, which were a mean of those of Hagai Netzer's ION and roughly version 76 of CLOUDY. The lines are generally still in good agreement with the predictions of that paper. In particular the changes in the line fluxes shown in Figure 1 of that paper are reproduced quite well.

---

blr_rnfb.in

table 1 of Rees et al. ApJ 347, 648

```
title table 1 of Rees et al. ApJ 347, 648
#
# blr model from
#
# commands controlling continuum =========
table agn
ionization parameter -2
#
# commands for density & abundances =========
hden 12
init file="c84.ini"
abundances he= -1 c= -3.328 n= -4.0088 o= -3.0809 ne= -4 na= -20
continue mg= -4.3768 al= -5.5686 si= -4.36653 s= -4.76955
continue ar= -5.4202 ca= -5.6383 fe= -4.4815 ni= -20
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
iterate to convergence
#
# commands controlling output =========
print line faint -1
print line optical depths
save performance "blr_rnfb.per"
save overview last "blr_rnfb.ovr"
save convergence reason last "blr_rnfb.cvr"
save element nitrogen last "blr_rnfb.nit"
save dr last "blr_rnfb.dr"
save results last "blr_rnfb.rlt"
save line emissivity "blr_rnfb.ems"
H 1 4861.32A
blnd 8446
blnd 1304
end of lines
normalize "H 1" 1215.67A = 91.8
#
# blr_rnfb.in
# class blr
# ======================================
#
```

This is a very dense cloud, and was computed in Rees et al. (1989). Table 1 of that paper lists the predictions, which were a mean of those of Hagai Netzer's ION and roughly version 76 of CLOUDY. The lines are generally still in good agreement with the predictions of that paper. In particular the changes in the line fluxes shown in Figure 1 of that paper are reproduced quite well. The fluxes of Lya and Hb are not reproduced with great precision by this model because of changes in collision rates for hydrogen and especially the form of the escape probability function for subordinate lines. As Figure 1 of RNF showed the line intensities are very sensitive to density for these parameters.

---

chianti_all_cool.in

cooling of a collisionally ionized plasma

```
title cooling of a collisionally ionized plasma
#
# commands controlling continuum =========
cosmic rays, background
coronal 4 vary
```

```
grid 4 6 0.5 sequential
database chianti "CloudyChiantiAll.ini" levels max
species "Fe+" levels=all
#
# commands for density & abundances =========
hden 0
set eden 0
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
#
# commands controlling output =========
save overview "chianti_all_cool.ovr"
save performance "chianti_all_cool.per"
save grid "chianti_all_cool.grd" last no hash
save cooling "chianti_all_cool.col" last no hash
save emitted continuum "chianti_all_cool.con" units angstroms
#
```

---

chianti_fe_cool.in

cooling of a collisionally ionized plasma

```
title cooling of a collisionally ionized plasma
#
# commands controlling continuum =========
cosmic rays, background
coronal 4 vary
database stout print
database chianti "CloudyChiantiFe.ini" print
species "Fe+" levels=all
grid 4 6 0.5 sequential
#
# commands for density & abundances =========
hden 0
init "honly.ini"
element iron on
element iron abundance 0
set eden 0
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
#
# commands controlling output =========
save overview "chianti_fe_cool.ovr"
save performance "chianti_fe_cool.per"
save grid "chianti_fe_cool.grd" last no hash
save cooling "chianti_fe_cool.col" last no hash
save emitted continuum "chianti_fe_cool.con" units angstroms
#
```

This tests the use of Chianti limited to Fe ions, and the Kurucz Fe III, IV, and V added by Matt Lykins

---

coll_coronal.in

model of active region of solar corona

```
title model of active region of solar corona
#
# commands controlling continuum =========
# temperature of corona
coronal equilibrium, 2.5e6 K
# assume the sun is a blackbody at 5770K
blackbody 5770 K
luminosity solar linear 1
#
# commands for density & abundances =========
hden log=10
#
# commands controlling geometry =========
# its height above photosphere and thickness
radius 11 thickness = 10
# the gas fully covers the center of symmetry
sphere
#
# other commands for details =========
iterate
#
# commands controlling output =========
normalize to "o 8" 18.9689A
save overview "coll_coronal.ovr"
save performance "coll_coronal.per"
save dr "coll_coronal.dr" last
save continuum "coll_coronal.con" last units angstroms
#
#
# coll_coronal.in
# class coronal
# ======================================
#
```

This is a rough model of the solar corona. The test checks that the coronal equilibrium commands work. The gas is predominantly collisionally ionized.

---

coll_heat_only.in

test code in limit where ONLY mechanical heating is present

```
title test code in limit where ONLY mechanical heating is present
#
# commands controlling continuum =========
no photoionization
blackbody 5000 STE
#
# commands controlling geometry =========
stop column density 15
#
# commands for density & abundances =========
hden 10
#
# other commands for details =========
hextra -1.5
iterate
#
# commands controlling output =========
# this command must be tested somewhere
print cooling, zone 5
# output files
save performance "coll_heat_only.per"
save overview "coll_heat_only.ovr"
save heating "coll_heat_only.het"
```

```
save cooling "coll_heat_only.col"
save convergence reason "coll_heat_only.cvr"
save dr "coll_heat_only.dr"
save continuum "coll_heat_only.con" units angstroms
#
#
# coll_heat_only.in
# class coronal
# ======================================
```

This test is an optically thin collisionally ionized gas with no photoionization at all.

---

coll_t3.in

coronal equilibrium at 10^3 K

```
title coronal equilibrium at 10^3 K
#
# commands controlling continuum =========
coronal 3
# add component of cosmic rays to drive chemistry
cosmic ray background
#
# other commands for details =========
iterate
#
# commands controlling geometry =========
stop column density 15
stop temperature off
#
# commands for density & abundances =========
hden 10
#
# other commands for details =========
# this sim needs very precise convergence to get a reliable result
set eden convergence tolerance 1e-4
#
# commands controlling output =========
save performance "coll_t3.per"
save overview "coll_t3.ovr"
save continuum "coll_t3.con" units angstroms
save dominant rates "coll_t3.sulphur" "S"
save dominant rates "coll_t3.molh2" "H2"
save dominant rates "coll_t3.molh" "H"
#
#
# coll_t3.in
# class coronal
# ======================================
```

This tests conditions of collisional equilibrium at low densities. This is one of a series of sims coll_t?.in which test ionization over a range of temperatures. This one, unlike the others, includes cosmic rays. Chemistry is important at this low temperature and the chemical network will collapse without a source of ionization. The cosmic rays provide this source of ionization.

---

coll_t3_grains.in

coronal equilibrium at 10^3 K, with grains to assist chemistry

```
title coronal equilibrium at 10^3 K, with grains to assist chemistry
```

```
#
# commands controlling continuum =========
coronal 1e3K
# add component of cosmic rays to drive chemistry
cosmic ray background
# >>chng 20 sep 19 test updated ISM abundances
abundances "ISM-HD20.abn"
set H2 Jura rate
#
# other commands for details =========
iterate
#
# commands controlling geometry =========
stop zone 1
#
# commands for density & abundances =========
hden 4
#
# other commands for details =========
# this sim needs very precise convergence to get a reliable result
set eden convergence tolerance 1e-4
#
# commands controlling output =========
save performance "coll_t3_grains.per"
save overview "coll_t3_grains.ovr"
save continuum "coll_t3_grains.con" units angstroms
#
#
# coll_t3_grains.in
# class coronal
# ======================================
```

This tests conditions of collisional equilibrium at low densities. This is one of a series of sims coll_t?.in which test ionization over a range of temperatures. This one, unlike the others, includes cosmic rays and grains. Chemistry is important at this low temperature and the chemical network will collapse without a source of ionization. The cosmic rays provide this source of ionization.

---

coll_t4.in

coronal equilibrium at 10^4 K

```
title coronal equilibrium at 10^4 K
#
# commands controlling continuum =========
coronal 4
#
# other commands for details =========
iterate
#
# commands controlling geometry =========
stop column density 15
#
# commands for density & abundances =========
hden 10
#
# commands controlling output =========
save performance "coll_t4.per"
save overview "coll_t4.ovr"
save continuum "coll_t4.con" units angstroms
#
#
# coll_t4.in
# class coronal
# ======================================
```

this tests conditions of collisional equilibrium at low densities

---

coll_t4_Z30.in

coronal equilibrium at 10^4 K

```
title coronal equilibrium at 10^4 K
#
# commands controlling continuum =========
coronal 4
#
# other commands for details =========
iterate
#
# commands controlling geometry =========
stop column density 15
#
# commands for density & abundances =========
hden 10
metals 30
#
# commands controlling output =========
save performance "coll_t4_Z30.per"
save overview "coll_t4_Z30.ovr"
save continuum "coll_t4_Z30.con" units angstroms
#
#
# coll_t4_Z30.in
# class coronal
# ======================================
```

This tests conditions of collisional equilibrium at low densities and high metallicity, where H-O CX will strongly affect ionization of H

This is the high Z mate to coll_t4.in

---

coll_t5.in

coronal equilibrium at 10^5 K

```
title coronal equilibrium at 10^5 K
#
# commands controlling continuum =========
coronal 5
#
# commands controlling geometry =========
stop column density 15
# test the luminosity case
radius 13
#
# commands for density & abundances =========
hden 10
#
# other commands for details =========
iterate
#
#
# commands controlling output =========
# normalize to strong HeII line
normalize to "He 2" 303.784A
save performance "coll_t5.per"
```

```
save overview "coll_t5.ovr"
save continuum "coll_t5.con" units angstroms
#
# coll_t5.in
# class coronal
# ======================================
```

This is a test collisional ionization equilibrium at 1e5 K.

---

coll_t6.in

coronal equilibrium at 10^6 K

```
title coronal equilibrium at 10^6 K
#
# commands controlling continuum =========
coronal 6
#
# commands controlling geometry =========
stop column density 15
#
# commands for density & abundances =========
hden 10
#
# other commands for details =========
iterate
#
# commands controlling output =========
normalize to "c 5" 40.2678A
# output files
save performance "coll_t6.per"
save overview "coll_t6.ovr"
save continuum "coll_t6.con" units angstroms
#
# coll_t6.in
# class coronal
# ======================================
```

This test is an optically thin collisionally ionized gas.

---

coll_t7.in

coronal equilibrium at 10^7 K

```
title coronal equilibrium at 10^7 K
#
# commands controlling continuum =========
coronal 7
#
# commands controlling geometry =========
stop column density 15
#
# commands for density & abundances =========
hden 10
#
# other commands for details =========
#
normalize to "o 8" 18.9689A
# commands controlling output =========
save performance "coll_t7.per"
save overview "coll_t7.ovr"
```

```
save continuum "coll_t7.con" units angstroms
save cooling "coll_t7.col"
save each cooling last "coll_t7.cole"
save cooling each "coll_t7.cle"
#
# coll_t7.in
# class coronal
# ======================================
```

Test with only collisional ionization at a high temperature.

---

dynamics_orion_flow.in

Orion nebula blister with wind

```
title Orion nebula blister with wind
#
# commands controlling continuum =========
blackbody 40000
phi(h) 13.0
brems 6
phi(h) 10
#
# commands for density & abundances =========
hden 4
abundances hii region no grains
grains orion no qheat single
#
# commands controlling geometry =========
wind -7 km/s advection
# this accounts for matter beyond end of the model
double optical depths
sphere
stop AV 5
stop temperature linear 5
#
# other commands for details =========
iterate 4
magnetic field -4
cosmic rays background
# this has no effect on dynamics, but is to desaturate the lines as per flow
turbulence 8 km/sec no pressure
# try to speed up simulation without hurting dynamics
init "fast.ini"
# use Bakes & Tielens heating
set PAH Bakes
#
# commands controlling output =========
# want to print line intensities are surface brightness, per arcsec^2
print lines surface brightness arcsec
print line faint -1.5
# the normalizing line is not defined on the emergent line stack
print lines emergent off
save performance "dynamics_orion_flow.per"
save overview "dynamics_orion_flow.ovr" no hash
save hydrogen 21 cm "dynamics_orion_flow.21cm" no hash
save dr "dynamics_orion_flow.dr" no hash
save continuum last "dynamics_orion_flow.con" units microns no hash
save pressure "dynamics_orion_flow.pre" no hash
save heating "dynamics_orion_flow.het" no hash
save cooling "dynamics_orion_flow.col" no hash
save molecules "dynamics_orion_flow.mol" no hash
save wind "dynamics_orion_flow.wnd" last
#
# dynamics_orion_flow.in
```

```
# class dynamics hii pdr
# ======================================
#
```

This is a model similar in spirit to the blister geometry H+ region model computed by Baldwin et al. (1991), but with a D-critical flow. Many physical processes have been disabled to make this simulationn faster. Grain physics is not done so the gas temperature is incorrect. The main purpose is to do a quick test of the dynamical flow with grain opacities included. The slow directory contains a full simulation of a flow like Orion.

---

dynamics_veryfast.in

very fast wind model

```
title very fast wind model
#
# commands controlling continuum =========
table agn
ionization parameter -2
#
# commands for density & abundances =========
hden 9
# this is a set of commands to speed up calc
init file "fast.ini"
#
# commands controlling geometry =========
stop thickness 8.4
# this is a subsonic wind with advection
wind velo -5 advection
#
# other commands for details =========
# absolutely no convergence problems should occur
failures 1
# this degrades the continuum resolution by factor of 3, to
# speed up calc
set continuum resolution 3
iterate 4
#
# commands controlling output =========
# the normalizing line is not defined on the emergent line stack
print lines emergent off
save overview "dynamics_veryfast.ovr"
save performance "dynamics_veryfast.per"
save pressure last "dynamics_veryfast.pre"
save total opacity last "dynamics_veryfast.opc"
save ionizing continuum last "dynamics_veryfast.ion"
save continuum last "dynamics_veryfast.con"
save dr "dynamics_veryfast.dr"
#
#
# dynamics_veryfast.in
# class dynamics
# ======================================
#
```

This is meant to be a very fast calculation to use when running extensive debug-enabled runtimes.

---

dynamics_veryfast_rec.in

very fast wind model

```
title very fast wind model
#
# commands controlling continuum =========
table agn
ionization parameter -2
#
# commands for density & abundances =========
hden 9
# this is a set of commands to speed up calc
init file "fast.ini"
#
# commands controlling geometry =========
stop thickness 8.4
# this is a subsonic wind with advection
wind velo 5 advection
#
# other commands for details =========
# absolutely no convergence problems should occur
failures 1
# this degrades the continuum resolution by factor of 3, to
# speed up calc
set continuum resolution 3
iterate 4
#
# commands controlling output =========
# the normalizing line is not defined on the emergent line stack
print lines emergent off
save overview "dynamics_veryfast_rec.ovr"
save performance "dynamics_veryfast_rec.per"
save pressure last "dynamics_veryfast_rec.pre"
save total opacity last "dynamics_veryfast_rec.opc"
save ionizing continuum last "dynamics_veryfast_rec.ion"
save continuum last "dynamics_veryfast_rec.con"
save dr "dynamics_veryfast_rec.dr"
#
#
# dynamics_veryfast_rec.in
# class dynamics
# ========================================
#
```

This is meant to be a very fast calculation to use when running extensive debug-enabled runtimes.

---

dynamics_wind.in

test of equations of motion in a very highly ionized wind

```
title test of equations of motion in a very highly ionized wind
#
# test motion in electron scattering limit
# radiative acceleration (e- only) is 9.54E-7 cm s^-2
# terminal velocity (e- only) is 7.6 km s^-1
#
# commands controlling continuum =========
table agn
luminosity (total) 45
#
# commands for density & abundances =========
hden 4
# this only includes H and He
init file="hheonly.ini"
#
# commands controlling geometry =========
radius (parsecs) 1
```

```
stop thickness (parsecs) -1
# a slow wind velocity, will assert velocity at outer radius
wind velo 0.1 ball
#
# other commands for details =========
# this will speed things up a bit
no level2
no radiation pressure
constant temperature 8
#
# commands controlling output =========
save overview "dynamics_wind.ovr"
save performance "dynamics_wind.per"
save pressure "dynamics_wind.pre"
save wind "dynamics_wind.wnd"
save dr "dynamics_wind.dr"
#
# dynamics_wind.in
# class limit dynamics
# ======================================
#
```

This tests the radiative acceleration and terminal velocity of a wind in which only electron scattering is important. The parameters were chosen so that electron scattering is the dominant opacity source, so that the equations can be solved both numerically (in the example) and analytically (the expected solution given above). In a realistic wind the gas would be more neutral and line driving would dominate. The force multiplier, given in the save wind output, is nearly unity as a result.

Checks:
- The radiative acceleration is correct (e- 9.543910-7 cm s-2).
- The terminal velocity should be 7.57 km s-1.
- Force multiplier near unity (no line driving since so highly ionized).
- Thickness of cloud correct (R-Ro + dr/2 should be 3.086391017 cm).

---

feii_hin.in

test feii in high density limit

```
title test feii in high density limit
#
# commands controlling continuum =========
black 25000 K
ionization -10
#
# commands for density & abundances =========
hden 18
# force a high electron density to insure collisions dominate
eden 18
#
# commands controlling geometry =========
constant tempera 4
stop zone 1
#
# other commands for details =========
species "Fe+" levels=all
iterate
# want to test collision only limit
no induced processes
#
# commands controlling output =========
set save prefix "feii_hin"
save overview ".ovr"
save performance ".per"
save species continuum ".fe2con" "Fe+" last units microns
```

```
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last
#
#
# feii_hin.in
# class limit
# ======================================
#
```

This checks that, at high particle densitites, in which the gas should be in collisional equilibrium, the level populations of the large model Fe+ ion go to the proper values, where the departure coefficients are all equal to unity.

---

feii_hirad.in

feii in case of high radiation density limit

```
title feii in case of high radiation density limit
#
# commands controlling continuum =========
black 8000 K lte
#
# commands for density & abundances =========
hden 9
element iron abundance 2
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
species "Fe+" levels=all
constant tempera 8000
iterate
#
# commands controlling output =========
set save prefix "feii_hirad"
save overview ".ovr"
save performance ".per"
save species densities ".lv1" "Fe+[:200]" last
save species densities ".lv2" "Fe+[201:]" last
save species continuum ".fe2con" "Fe+" last units microns
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last
#
#
# feii_hirad.in
# class limit
# ======================================
#
```

This checks that, at high radiation densitites, in which the gas is irradiated by a blackbody in strict thermodynamic equilibrium, the level populations of the large model Fe+ ion go to the proper values, where the departure coefficients are all equal to unity.

---

feii_pump.in

test feii in continuum pumped limit

```
title test feii in continuum pumped limit
#
# commands controlling continuum =========
black 25000 K
```

```
ionization -5
#
# commands for density & abundances =========
hden 10
abundances old solar 84
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
Case B
iterate
constant tempera 4
species "Fe+" levels=all
#
# commands controlling output =========
set save prefix "feii_pump"
save overview ".ovr"
save performance ".per"
save species continuum ".con" "Fe+" units microns last
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last
#
#
# feii_pump.in
```

This is a constant temperature low ionization cloud, with BLR-like densities, which includes the large FeII atom. The tests check on the emission predicted in the Fe II bands.

This model tests the large FeII model in the optically thin, continuum pumped limit. The zone thickness is set to a small value (1 cm) so that full continuum hits atom.

---

feii_ste.in

thermal equilibrium of FeII in STE limit

```
title thermal equilibrium of FeII in STE limit
#
# commands controlling continuum =========
black 8000 K lte
hden 9
#
# commands for density & abundances =========
element iron abundance 2
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
species "Fe+" levels=all
iterate
#
# commands controlling output =========
set save prefix "feii_ste"
save overview ".ovr"
save performance ".per"
save continuum last ".con"
save species column density last ".col" "Fe+"
save species densities last ".pop" "Fe+[:]"
save species departure last ".dep" "Fe+[:]"
save species levels last ".lev" "Fe+"
save species continuum ".fe2con" "Fe+" last units microns
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last
#
# feii_ste.in
```

```
# class function
# ======================================
#
```

This model has a very high iron abundance, 100x H, and most Fe is in the form of Fe+. It is irradiated by a blackbody in strict thermodynamic equilibrium. We check that the temperature of the gas is equal to the radiation temperature, to confirm that the thermal properties of the model FeII atom obey thermodynamics.

---

feii_t4n0.in

FeII emission in typical intermediate density photoionzied cloud

```
title FeII emission in typical intermediate density photoionzied cloud
#
# commands controlling continuum =========
black 5e5K
ionization parameter -2
#
# commands for density & abundances =========
hden 0
element iron abundance 2
element iron ionization -7 0 -7
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature 4
species "Fe+" levels=all
#
# commands controlling output =========
print lines column
print line inward
print line sort wavelength
print line faint 0.1
normalize "Fe 2b" 5270
set save prefix "feii_t4n0"
save overview ".ovr"
save performance ".per"
save species continuum last ".con" "Fe+" units angstroms
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last no hash
#
#
# feii_t4n0.in
# class function
# ======================================
#
```

This model has a very high iron abundance, 100x H, and most Fe is in the form of Fe+. it has a low density and unit thickness

The model is optically thin, no RT.

---

feii_t4n8.in

FeII emission in typical intermediate density photoionzied cloud

```
title FeII emission in typical intermediate density photoionzied cloud
#
```

```
# commands controlling continuum =========
black 5e5K
ionization parameter -2
#
# commands for density & abundances =========
hden 8
element iron abundance 2
element iron ionization -7 0 -7
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature 4
species "Fe+" levels=all
#
# commands controlling output =========
print lines column
print line inward
print line sort wavelength
print line faint 0.1
normalize "Fe 2b" 5270
set save prefix "feii_t4n8"
save overview ".ovr"
save performance ".per"
save species continuum last ".con" "Fe+" units angstroms
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last no hash
#
#
# feii_t4n8.in
# class function
# ======================================
#
```

This model has a very high iron abundance, 100x H, and most Fe is in the form of Fe+. it has a low density and unit thickness

The model is optically thin, no RT.

---

feii_t4n8_rt.in

FeII emission in typical intermediate density photoionzied cloud

```
title FeII emission in typical intermediate density photoionzied cloud
#
# commands controlling continuum =========
black 5e5K
ionization parameter -2
#
# commands for density & abundances =========
hden 8
element iron abundance 2
element iron ionization -7 0 -7
#
# commands controlling geometry =========
stop thickness 5
#
# other commands for details =========
constant temperature 4
species "Fe+" levels=all
iterate 3
#
# commands controlling output =========
print line precision 6
```

```
print lines column
print line inward
print line sort wavelength
print line faint 0.1
normalize "Fe 2b" 5270
set save prefix "feii_t4n8_rt"
save overview ".ovr"
save performance ".per"
save species continuum last ".con" "Fe+" units angstroms
save species inward continuum last ".cin" "Fe+" units angstroms
save species outward continuum last ".cout" "Fe+" units angstroms
save species column density last ".col" "Fe+[:]"
save species densities last ".pop" "Fe+[:]"
save species optical depth last ".opt" "Fe+"
save species lines last ".lin" "Fe+"
save species bands ".fe2b" "FeII_bands.dat" "Fe+"
save line emissivity ".ems"
"Fe 2b" 2797
"Fe 2b Inwd" 2797
end of lines
#
#
# feii_t4.in
# class function
# ======================================
#
```

This model has a very high iron abundance, 100x H, and most Fe is in the form of Fe+. it has intermediate density and should produce and FeII spectrum something like an AGN. The set line precision 6 increases the number of significant figures in the wavelengths for each line. This is needed to get the right FeII inward band.

This has a finite thickness and so tests the RT, line overlap.

---

feii_t4n8_Smyth19.in

FeII emission in typical intermediate density photoionzied cloud

```
title FeII emission in typical intermediate density photoionzied cloud
species "Fe+" dataset="Smyth19"
database Stout print
#
# commands controlling continuum =========
black 5e5K
ionization parameter -2
#
# commands for density & abundances =========
hden 8
element iron abundance 2
element iron ionization -7 0 -7
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature 4
species "Fe+" levels=all
#
# commands controlling output =========
print lines column
print line inward
print line sort wavelength
print line faint 0.1
normalize "Fe 2b" 5270
set save prefix "feii_t4n8_Smyth19"
```

```
save overview ".ovr"
save performance ".per"
save species continuum last ".con" "Fe+" units angstroms
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last no hash
#
#
# feii_t4n8_Tayal18.in
# class function
# ======================================
#
```

This model has a very high iron abundance, 100x H, and most Fe is in the form of Fe+. it has a low density and unit thickness

The model is optically thin, no RT.

---

feii_t4n8_Tayal18.in

FeII emission in typical intermediate density photoionzied cloud

```
title FeII emission in typical intermediate density photoionzied cloud
species "Fe+" dataset="Tayal18"
database Stout print
#
# commands controlling continuum =========
black 5e5K
ionization parameter -2
#
# commands for density & abundances =========
hden 8
element iron abundance 2
element iron ionization -7 0 -7
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature 4
species "Fe+" levels=all
#
# commands controlling output =========
print lines column
print line inward
print line sort wavelength
print line faint 0.1
normalize "Fe 2b" 5270
set save prefix "feii_t4n8_Tayal18"
save overview ".ovr"
save performance ".per"
save species continuum last ".con" "Fe+" units angstroms
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last no hash
#
#
# feii_t4n8_Tayal18.in
# class function
# ======================================
#
```

This model has a very high iron abundance, 100x H, and most Fe is in the form of Fe+. it has a low density and unit thickness

The model is optically thin, no RT.

---

feii_t4n8_Verner99.in

FeII emission in typical intermediate density photoionzied cloud

```
title FeII emission in typical intermediate density photoionzied cloud
species "Fe+" dataset="Verner99"
database Stout print
#
# commands controlling continuum =========
black 5e5K
ionization parameter -2
#
# commands for density & abundances =========
hden 8
element iron abundance 2
element iron ionization -7 0 -7
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature 4
species "Fe+" levels=all
#
# commands controlling output =========
print lines column
print line inward
print line sort wavelength
print line faint 0.1
normalize "Fe 2b" 5270
set save prefix "feii_t4n8_Verner99"
save overview ".ovr"
save performance ".per"
save species continuum last ".con" "Fe+" units angstroms
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last no hash
#
#
# feii_t4n8_Tayal18.in
# class function
# ======================================
#
```

This model has a very high iron abundance, 100x H, and most Fe is in the form of Fe+. it has a low density and unit thickness

The model is optically thin, no RT.

---

func_abund_fluc.in

check fluctuating heavy-element abundances

```
title check fluctuating heavy-element abundances
# commands controlling continuum =========
blackbody 5
ionization -2
#
# commands for density & abundances =========
hden 3
# this varies the abundnaces between default and 1e-4 times default,
# over a 1e10 cm period - we will compute half a cycle
fluctuations abundances 10.3 0 -4
```

```
#
# commands controlling geometry =========
# stop at half a cycle so pick off lowest abundances
stop thickness 10
#
# other commands for details =========
# speed things up a bit
init "c84.ini"
#
# commands controlling output =========
print column density
save performance "func_abund_fluc.per"
save overview "func_abund_fluc.ovr"
save abundances "func_abund_fluc.abn"
#
# commands giving asserts
#
# func_abund_fluc.in
# class function
# ======================================
#
```

This checks that the variable abundances option works

---

func_distance.in

check that distance and "print flux earth" commands work

```
title check that distance and "print flux earth" commands work
#
# commands controlling continuum =========
# luminosity in ionizing radiation, this and distance
# were chosen so that flux at earth assocated with total
# luminoisity of object is 1 erg cm-2 s-1
luminosity 40
laser 2
#
# must test capabiliites somewhere
# >>19 07 09, add abundances
abundances "palme14-Sol.abn"
#
# commands for density & abundances =========
hden 4
# >>19 07 09, add abundances
# init file "honly.ini"
#
# commands controlling geometry =========
stop zone 1
radius 17
#
# other commands for details =========
distance 19.450395
constant temperature 4
#
# commands controlling output =========
# give flux at Earth
print lines, flux at Earth
save overview "func_distance.ovr"
save performance "func_distance.per"
#
# func_distance.in
# class function
# ======================================
#
```

Normally the code predicts the intensity or luminosity of the emission lines. This test confirms that it can predict the flux recieved at the Earth instead. The model is the simplest and fastest that can be computed - a H-only constant temperature single zone. The total luminosity is set to 1e40 erg/s, and the ionization source is a laser at 2 ryd. With these set, the total luminosity in ionizing radiation, the total luminoisity in the incident continuum (the emission line labeled "Inci 0") will be 1e40.

The code will predict the flux at the Earth if both the distance to the oject is specified with the distance command, and this is requested with the print flux earth command. The distance was chosen so that the total flux at the Earth will be 1 erg/s. This is asserted at the end of the calculation.

---

func_dlaw.in

test model with dlaw table

```
title test model with dlaw table
#
# commands controlling continuum =========
phi(H) 15
table agn
#
# commands for density & abundances =========
dlaw table radius
continue 16 9
continue 17 7
continue 18 5
continue 19 3
continue 20 1
continue 21 -1
end of dlaw
#
# must test capabiliites somewhere
# >>19 07 09, add abundances
abundances "palme14-Met.abn"
#init "honly.ini"
#
# commands controlling geometry =========
sphere
filling factor -5
radius 17 20
#
# other commands for details =========
constant temperature 4
#
# commands controlling output =========
save overview "func_dlaw.ovr"
save performance "func_dlaw.per"
save dr "func_dlaw.dr"
save overveiw "func_dlaw.ovr"
#
#
# func_dlaw.in
# class function
# ======================================
#
```

this model tests the dlaw density table command

---

func_fulltrace.in

test full trace output

```
title test full trace output
#
# commands controlling continuum =========
trace h-like hydrogen full no print
# check that no uninitialized rates are printed (r2757)
print arrays ionization carbon only
print arrays levels "C[1:5]"
stop zone 1
table agn
ionization parameter -0.5
#
# commands for density & abundances =========
hden 9.5
init file="honly.ini"
element carbon on
#
# other commands for details =========
database h-like element hydrogen collapsed levels 1
#
# commands controlling output =========
# func_fulltrace.in
# class function
# ======================================
```

this checks that trace output functions correctly

---

func_globule.in

test of globule command

```
title test of globule command
#
# commands controlling continuum =========
black 40000 K
ionization parameter -1.5
#
# commands for density & abundances =========
globule initial density=5 scale depth=14
init file "ism.ini"
abundances hii region no qheat
#
# commands controlling geometry =========
#
# other commands for details =========
failures 2
#
# commands controlling output =========
print line faint -1.5
save performance "func_globule.per"
save overview last "func_globule.ovr"
save results last "func_globule.rlt"
save dr "func_globule.dr" last
save heating "func_globule.het" last
save cooling "func_globule.col" last
#
# func_globule.in
# class function
# ======================================
#
```

This model uses the globule command, tests that the zoning logic works for this extreme case, and that the code is able to converge the globule model.

---

func_grid_line_ratios.in

test generating line ratios in a grid run

```
title test generating line ratios in a grid run
#
# commands controlling continuum =====
blackbody 4e4 K
ionization parameter -2
#
# commands for density & abundances =====
# these are to speed up the calculation, only do H, O, and Ne
init "honly.ini"
element oxygen on
element neon on
element sulphur on
element oxygen ionization 1 1 1
element neon ionization 1 1 1
element sulphur ionization 1 1 1
# vary the hydrogen density
hden 4 vary
grid 2 6.1 1 sequential
#
# other commands for details =======
# these are constant temperature models, vary T
constant temperature 4 vary
grid 4000 17000 3000 linear
stop zone 1
#
# commands controlling output =====
save overview "func_grid_line_ratios.ovr"
save performance "func_grid_line_ratios.per"
save line list "func_grid_line_ratios.pun" "func_grid_line_ratios.dat" ratio no hash
save grid "func_grid_line_ratios.grd"
#
# commands giving (lack of) assert ==========
#
# func_grid_line_line_ratios.in
# class function
# ================================================
```

This uses the grid command to compute line ratios for a wide range of density and temperature. The ionization is set to a uniform value and only a few elements are included. this makes the calculation faster and prevents recombination [O III] 4363 from becoming important (there is no O+3).

These are the line ratios mentioned as limits in the Johnstone et al. Spitzer cooling flow filament paper (2007).

---

func_grid_list.in

test the 'list' keyword on the grid command

```
title test the 'list' keyword on the grid command
blackbody 10000 STE vary
grid list "func_grid_list.dat" linear sequential
hden 5
stop zone 1
iterate 2
***************
```

This is a simple grid with parameter values stored in an external file. That file is also used to monitor the temperature of each grid point.

func_hotgas_coolstar.in

test very soft continuum, very hot gas

```
title test very soft continuum, very hot gas
#
# commands controlling continuum =========
# put in the cosmic background as the only continuum source
CMB
# gas has constant temperature of 1e6 K
constant temperature, t=6
#
# commands for density & abundances =========
hden 10.
#
# commands controlling geometry =========
stop zone 1
# specify a thin cell of gas - 1 cm thick
set dr 0
#
# other commands for details =========
# iterate since gas is optically thin
iterate
#
# commands controlling output =========
save overview "func_hotgas_coolstar.ovr"
save performance "func_hotgas_coolstar.per"
#
# func_hotgas_coolstar.in
# class limit
# ======================================
#
```

This is a test where the CMB is the only continuum source. It does not extend to energies where the code needs to work. There are special cases used in this situation, for continuum addressing, so this checks whether those still function.

---

func_ion_increase.in

test model where ionization increases with depth

```
title test model where ionization increases with depth
#
# commands controlling continuum =========
ionization parameter -4
table agn
#
# commands for density & abundances =========
hden 7 -4
init "hheonly.ini"
element oxygen on
element iron on
#
# commands controlling geometry =========
sphere
filling factor -5
radius 17 20
#
# other commands for details =========
constant temperature 4
#
# commands controlling output =========
```

```
save overview "func_ion_increase.ovr"
save performance "func_ion_increase.per"
save dr "func_ion_increase.dr"
save overveiw "func_ion_increase.ovr"
save element oxygen "func_ion_increase.oxy"
save element iron "func_ion_increase.fe"
#
#
# func_ion_increase.in
# class function
# ======================================
#
```

This density falls off faster than 1/r^2 so the ionization increases with depth. Most sims have decreasing rather than increasing ionization.

---

func_iso_large.in

test large iso sequence model atom

```
title test large iso sequence model atom
#
# commands controlling continuum =========
blackbody 5e4
ionization parameter -2
CMB
#
# commands for density & abundances =========
hden = 2.3
eden = 2.3
metals .3 log
#
# commands controlling geometry =========
sphere
stop zone 10
#
# other commands for details =========
database H-like levels large element hydrogen
database He-like levels large element helium
#
# commands controlling output =========
print every 1
database H-like levels print
save performance "func_iso_large.per"
save dr "func_iso_large.dr"
save overview "func_iso_large.ovr"
save line labels "func_iso_large.lbl"
#
#
# func_iso_large.in
# class function
# ======================================
#
```

this model tests the large model atoms for the iso sequences. the large models are used for H I and He I. monitor lines from both low-lying and Rydberg levels to test the full model. the lines from Rydberg states as well as the He I 10830 line are ambiguous so this also exercises line disambiguation

---

func_LineList_BLR.in

```
test
```

```
print line precision 6
table lines "LineList_BLR.dat"
```

---

func_LineList_BLR_Fe2.in

```
test
print line precision 6
table lines "LineList_BLR_Fe2.dat"
set save prefix "func_LineList_BLR_Fe2"
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last
```

---

func_LineList_BLR_Fe2_vacuum.in

```
test
print line precision 6
print lines vacuum
table lines "LineList_BLR_Fe2.dat"
set save prefix "func_LineList_BLR_Fe2"
save species bands ".fe2b" "FeII_bands.dat" "Fe+" last
```

---

func_LineList_BLR_vacuum.in

```
test
print line precision 6
print lines vacuum
table lines "LineList_BLR.dat"
```

---

func_LineList_He_like.in

```
test
print line precision 6
table lines "LineList_He_like.dat"
```

---

func_LineList_He_like_vacuum.in

```
test
print line precision 6
print lines vacuum
table lines "LineList_He_like.dat"
```

---

func_LineList_HeH.in

```
test
print line precision 6
table lines "LineList_HeH.dat"
```

---

func_LineList_HeH_vacuum.in

```
test
print line precision 6
```

```
print lines vacuum
table lines "LineList_HeH.dat"
```

---

func_LineList_HII.in

```
test
print line precision 6
table lines "LineList_HII.dat"
```

---

func_LineList_HII_vacuum.in

```
test
print line precision 6
print lines vacuum
table lines "LineList_HII.dat"
```

---

func_LineList_NLR.in

```
test
print line precision 6
table lines "LineList_NLR.dat"
```

---

func_LineList_NLR_vacuum.in

```
test
print line precision 6
print lines vacuum
table lines "LineList_NLR.dat"
```

---

func_LineList_PDR.in

check that wavelengths agree at high line precision

```
title check that wavelengths agree at high line precision
test
print line precision 6
table lines "LineList_PDR.dat"
```

---

func_LineList_PDR_H2.in

check that wavelengths agree at high line precision

```
title check that wavelengths agree at high line precision
test
database h2
print line precision 6
table lines "LineList_PDR_H2.dat"
```

---

func_LineList_PDR_H2_vacuum.in

check that wavelengths agree at high line precision

```
title check that wavelengths agree at high line precision
test
database h2
print line precision 6
print lines vacuum
table lines "LineList_PDR_H2.dat"
```

---

func_LineList_PDR_vacuum.in

check that wavelengths agree at high line precision

```
title check that wavelengths agree at high line precision
test
print line precision 6
print lines vacuum
table lines "LineList_PDR.dat"
```

---

func_LineList_strong.in

```
test
print line precision 6
table lines "LineList_strong.dat"
```

---

func_LineList_strong_vacuum.in

```
test
print line precision 6
print lines vacuum
table lines "LineList_strong.dat"
```

---

func_lines.in

create output file with list of func_lines

```
title create output file with list of func_lines
print line precision 6
database h2 levels large
species "Fe+" levels=all
# report all species in use
database print
test
#
# commands controlling continuum =========
# commands for density & abundances =========
# commands controlling geometry =========
# other commands for details =========
#
# commands controlling output =========
# this creates the file "func_lines.lab" that contains a list
```

```
# of all emission labels
save overview "func_lines.ovr"
save performance "func_lines.per"
save line labels "func_lines.lab"
# the save species xxx series of line-related reports
save species labels "func_lines.spclab" all
save species lines "func_lines.spclin" all
save species levels units wavenumber "func_lines.spclev" all
# this must come last since code stops after doing it
# this creates the file "func_lines.lis" that contains a list
# of the emission func_lines that are transported.
save line data "func_lines.lis"
#
# There is nothing extra to assert, since test does include many asserts
#
# func_lines.in
# class function
# ======================================
#
```

This runs the standard "test" case, and then creates the line data and labels files. Test by itself includes many asserts, so no further asserts are needed here.

The file func_lines.lab is a useful list of all lines predicted by the code. Cut and paste this into other places when you need to find a particular emission line.

The func_lines lines.dat gives atomic data for all the lines, and their critical density at 10000 K. The large H2 and Fe II model atoms are turned on to include their lines.

---

func_ly_pump_scale.in

test scaling of H lyman-line pumping

```
title test scaling of H lyman-line pumping
sphere
blackbody 30000
q(h) 47
hden 2.5
radius 16
stop zone 1
database H-like Lyman pumping scale .2
```

This purpose of this test is just to exercise the option to scale the H lyman series pumping rates by some factor.

---

func_map.in

map of heating vs cooling

```
title map of heating vs cooling
#
# commands controlling continuum =========
table agn
ionization parameter -2.5
#
# commands for density & abundances =========
hden 0
abundances old solar 84
#
# commands controlling geometry =========
set dr 0
```

```
stop lyman optical depth -7
stop zone 1
#
# other commands for details =========
#
# commands controlling output =========
# save map information to generate plot for hazy
save overview "func_map.ovr"
save performance "func_map.per"
save map file="func_map.dta"
set nmaps 100
#
# map.in
# class function
# ======================================
#
```

This is a test of the continuity of the code over a very large range of temperature. It was used to produce one of the thermal maps shown in Hazy.

Checks:
- No breaks in the heating and cooling curves where various approximations change.

---

func_nolight.in

check OK with no radiation incident

```
title check OK with no radiation incident
constant temp 5e7 linear
hden 7 log
set dr 0
stop zone 1
#
save performance "func_nolight.per"
save dr "func_nolight.dr"
save overveiw "func_nolight.ovr"
#
#
# func_nolight.in
# class function
# ======================================
#
```

Check that we handle limit where there is no incident radiation field

---

func_sdrmin.in

test set drmin command

```
title test set drmin command
#
# commands controlling continuum =========
blackbody 8e4
luminosity 37.5
#
# commands for density & abundances =========
hden 4
#
# commands controlling geometry =========
```

```
radius 17
sphere
stop thickness 17.03
stop temperature off
#
# other commands for details =========
set drmin 15.5
cosmic rays background
#
# commands controlling output =========
save overview "func_sdrmin.ovr"
save performance "func_sdrmin.per"
save dr "func_sdrmin.dr" last
#
```

This simulation tests the SET DRMIN command. It is a toy model of a planetary nebula that is designed to extend into the PDR. The minimum stepsize is deliberately set much too large so that we would immediately notice if the command was broken. It also tests if we still hit the correct outer radius when SET DRMIN is used. Without the SET DRMIN command this sim would need 410 zones (trunk@2760).

---

func_set_ion.in

test impact of setting ionization

```
title test impact of setting ionization
#
# commands for density & abundances =========
init "ism.ini"
hden 0
element hydrogen ionization 0 1
element helium ionization 0 1 0
element carbon ionization 0 1
element oxygen ionization 0 0.1 0.2 0.3 0.2 0.1 0.1
element iron ionization -9 -9 -9 -9 -9 -9 -9 -9 -9 -9 -9 -9 0 -9 -9
#
# commands controlling continuum =========
blackbody 5
ionization parameter -2
#
# commands controlling geometry =========
# force model to be 1 cm thick
set dr 0
#
# other commands for details =========
constant temperature 4
stop zone 1
#
# commands controlling output =========
#>>chng 23 oct 13 add this command to test somewhere in tsuite
print lines vacuum
normalize to "o 3" 5006.84 air
save overview "func_set_ion.ovr"
save performance "func_set_ion.per"
save dr "func_set_ion.dr"
#
#
# func_set_ion.in
```

class function # ========== # this script exercies the option to specify the ionization of a species

---

func_stopcol.in

test stop column density "species" command

```
title test stop column density "species" command
#
# commands controlling continuum =========
ionization parameter -2
blackbody 50000
#
# commands for density & abundances =========
hden 2
init file "ism.ini"
# test option to turn off elements with small abundances
element limit off -5
#
# commands controlling geometry =========
# stop calc at line ratio, the point of this test
stop column density "N+2" 10.
#
# other commands for details =========
constant temperature 10000 K
#
# commands controlling output =========
set save prefix "func_stopcol"
save overview ".ovr"
save performance ".per"
save dr ".dr" last
#
#
#
#
# func_stopcol.in
# class function
# ======================================
#
```

This is an example of a simple calculation that stops when a column density of a species reaches a specific value. The tricky part is that the species label contains a number, so we need to ascertain that the column density is parsed correctly.

---

func_stopline1.in

test stop line command

```
title test stop line command
#
# commands controlling continuum =========
ionization parameter -2
blackbody 50000
#
# commands for density & abundances =========
hden 2
abundances old solar 84
init file "ism.ini"
# test option to turn off elements with small abundances
element limit off -5
#
# commands controlling geometry =========
# stop calc at line ratio, the point of this test
stop line "c 2" 157.636m reaches 0.0358
#
# other commands for details =========
constant temperature 10000 K
#
# commands controlling output =========
```

```
save overview "func_stopline1.ovr"
save performance "func_stopline1.per"
save dr "func_stopline1.dr" last
#
# func_stopline1.in
# class function
# ======================================
#
```

This is an example of a simple calculation that stops when a line reaches a specified intensity. The option to turn off elements with trivial abundances is used.

---

func_stopline2.in

test stop line command

```
title test stop line command
#
# commands controlling continuum =========
ionization parameter -2
blackbody 50000
#
# commands for density & abundances =========
hden 2
abundances old solar 84
init file "ism.ini"
#
# commands controlling geometry =========
# stop calc at line ratio, the point of this test
stop line "c 2" 157.636m air reaches 0.002 relative to "o 3" 5008.24 vacuum
#
# other commands for details =========
constant temperature 10000 K
#
# commands controlling output =========
normalize to "o 3" 5006.84
save overview "func_stopline2.ovr"
save performance "func_stopline2.per"
save dr "func_stopline2.dr" last
#
# func_stopline2.in
# class function
# ======================================
#
```

this is an example of a simple calculation that stops when a certain emission line ratio is reached

---

func_t10.in

test very soft continuum, very hot gas

```
title test very soft continuum, very hot gas
#
# commands controlling continuum =========
table agn
ionization parameters -2
#
# commands for density & abundances =========
hden 1.
#
# commands controlling geometry =========
```

```
stop zone 1
# specify a thin cell of gas - 1 cm thick
set dr 0
#
# other commands for details =========
# set constant temperature to high-T limit
constant temperature, t=10 log
# iterate since gas is optically thin
iterate
#
# commands controlling output =========
save overview "func_t10.ovr"
save performance "func_t10.per"
#
#
# func_t10.in
# class limit
# ======================================
#
```

This is a test of the highest temperature the code can do.

---

func_t3.in

test low temperature limit of code, 3K

```
title test low temperature limit of code, 3K
#
# commands controlling continuum =========
table agn
ionization parameters -2
#
# commands for density & abundances =========
hden -1
#
# commands controlling geometry =========
stop zone 1
# specify a thin cell of gas 1 cm thick
set dr 0
#
# other commands for details =========
# set constant temperature to low-T limit
constant temperature, t=3.0 linear
# iterate since gas is optically thin
iterate
#
# commands controlling output =========
save overview "func_t3.ovr"
save performance "func_t3.per"
#
#
#
# func_t3.in
# class limit
# ======================================
#
```

This is a test of the lowest temperature the code can do. It runs a constant temperature of 3K

---

func_t3_linesintroff.in

test low temperature limit of code, 3K

```
title test low temperature limit of code, 3K
#
# commands controlling continuum =========
table agn
ionization parameters -2
#
# commands for density & abundances =========
hden -1
#
# commands controlling geometry =========
stop zone 1
# specify a thin cell of gas 1 cm thick
set dr 0
#
# other commands for details =========
# set constant temperature to low-T limit
constant temperature, t=3.0 linear
# iterate since gas is optically thin
iterate
#
# commands controlling output =========
print lines intrinsic off
set save prefix "func_t3_linesintroff"
save overview ".ovr"
save performance ".per"
#
#
#
# func_t3.in
# class limit
# ========================================
#
```

This is a test of the lowest temperature the code can do. It runs a constant temperature of 3K. The predicted intrinsic spectrum is suppressed in the main output.

---

func_t3_linesoff.in

test low temperature limit of code, 3K

```
title test low temperature limit of code, 3K
#
# commands controlling continuum =========
table agn
ionization parameters -2
#
# commands for density & abundances =========
hden -1
#
# commands controlling geometry =========
stop zone 1
# specify a thin cell of gas 1 cm thick
set dr 0
#
# other commands for details =========
# set constant temperature to low-T limit
constant temperature, t=3.0 linear
# iterate since gas is optically thin
iterate
#
# commands controlling output =========
print lines off
set save prefix "func_t3_linesoff"
save overview ".ovr"
```

```
save performance ".per"
#
#
#
# func_t3.in
# class limit
# ======================================
#
```

This is a test of the lowest temperature the code can do. It runs a constant temperature of 3K. The predicted spectra (intrinsic and emergent) are suppressed in the main output.

---

func_test.in

run smoke test

```
title run smoke test
# commands controlling continuum =========
test
# commands for density & abundances =========
# commands controlling geometry =========
# other commands for details =========
# include this in one test to make sure it works
set continuum shield ferland
#
# commands controlling output =========
# increase precision of all printed wavelengths
print line precision 6
# following will print physical constants used by the code
print constants
# print RR and DR rates
print recombination
# the citation for the current version of the code
print citation
# following prints column densities
print column density
save performance "func_test.per"
save continuum "func_test.con"
save overview "func_test.ovr"
# func_test.in
# class function
# ======================================
#
```

This runs the smoke test command, which include several asserts. The tests the behavior of increasing the number of significant figures in printed wavelengths.

---

func_test_cycle.in

exercise full range of density, temperature

```
title exercise full range of density, temperature
#
# modified from slow/grid_extreme.in
# this version cycles through the corner models twice
# to see if the second repetition exactly matches the first
# checkall.pl calls test_grid.pl to check that output is identical
#
element lithium off
element berylium off
element boron off
```

```
cosmic rays background linear 0.1266
cmb
iterate
#
blackbody 6
energy density 6 vary
grid 1 6 5 cycle sequential
# -8 18
hden 2 vary
grid -6 15 21
stop zone 1
# set to constant small thickness
set dr -10
#
trace h-like full helium no print
trace he-like full no print
trace heavy no print
trace convergence esource no print
no time
#
save performance no hash "func_test_cycle.per"
save grid no hash "func_test_cycle.grd" last
save overview last no hash "func_test_cycle.ovr" last
save average "func_test_cycle.avr" last
temperature hydrogen 2
end of average
#
#
# func_test_cycle.in limits
```

---

func_test_grid.in

test whether the output from a repeated model reproduces exactly

```
title test whether the output from a repeated model reproduces exactly
print depart he-like element helium
trace h-like full helium no print
trace he-like full no print
trace heavy no print
trace convergence esource no print
test
no time
fudge 0 vary
grid 0 to 1 1 repeat sequential
iterate 3
***************
```

This tests that the code gets repeatable results in a large grid run. It will not if variables are not properly initialized. tsuite / programs / comp does a similar test.

auto / checkall.pl includes test to check this.

---

func_testmole.in

this runs the standard, one command, test, which contains many asserts

```
title this runs the standard, one command, test, which contains many asserts
# commands controlling continuum =========
test mole
#
# commands for density & abundances =========
```

```
# commands controlling geometry =========
# other commands for details =========
#
# commands controlling output =========
save performance "func_testmole.per"
save overview "func_testmole.ovr"
# func_testmole.in
# class function
# ======================================
#
```

This runs the "test mole" command, which include several asserts.

---

func_tlaw.in

test model with tlaw table

```
title test model with tlaw table
#
# commands controlling continuum =========
phi(H) 15
table agn
#
# commands for density & abundances =========
hden 9
init "honly.ini"
#
# commands controlling geometry =========
sphere
filling factor -5
radius 16 17
stop temperature 3 linear
#
# other commands for details =========
tlaw table radius
continue -35 4
continue 16 4
continue 16.2 3
continue 16.4 4
continue 16.6 3.5
continue 16.8 4
continue 20 4
continue 21 -1
end of tlaw
#
# commands controlling output =========
save overview "func_tlaw.ovr"
save performance "func_tlaw.per"
save dr "func_tlaw.dr"
save overveiw "func_tlaw.ovr"
#
#
# func_tlaw.in
# class function
# ======================================
#
```

this model tests the tlaw density table command

---

func_trans_lumi.in

test transmitted continuum in luminosity mode

```
title test transmitted continuum in luminosity mode
#
# common commands
init file "func_trans_lumi.dat"
#
# commands controlling geometry =========
radius 21
#
# commands controlling output =========
set save prefix "func_trans_lumi"
save overview ".ovr"
save performance ".per"
save ionization last ".ion"
save continuum last ".con"
#
# this contains a large number of asserts that both tests use
init file "trans_lumi.dat"
#
# func_trans_lumi.in
# class function
# ======================================
#
```

func_trans_lumi, func_trans_save_lumi, and func_trans_read_lumi_scale are a set of tests that check that the code can save a transmitted continuum in luminosity mode and then read it back in.

func_trans_lumi.in: this sim is directly illuminated by a BB at Rin = 1e21. Its predictions should be identical to func_trans_read_lumi_scale.in.

func_trans_save_lumi.in: this sim is directly illuminated by a BB at Rin = 1e20. It saves the transmitted continuum and has no monitors.

func_trans_read_lumi_scale.in: this sim is illiminated by the transmitted continuum at Rin = 1e21. Its predictions should be almost identical to func_trans_lumi.in. This tests that the transmitted continuum works correctly in luminosity mode and also that spherical dilution is handled correctly.

---

func_trans_read.in

second of func_trans_save/func_trans_read pair, use transmitted continuum

```
title second of func_trans_save/func_trans_read pair, use transmitted continuum
# the transmitted continuum produced by func_trans_punch
#
# commands controlling continuum =========
ionization parameter -1
table read "func_trans_save.trn"
brems 6
ionization parameter -6
#
# commands for density & abundances =========
hden 10
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
iterate
#
# commands controlling output =========
# this contains a large number of asserts used by both commands
init file "trans.dat"
save overview "func_trans_read.ovr"
```

```
save performance "func_trans_read.per"
save ionization last "func_trans_read.ion"
#
#
# func_trans_read.in
# class function
# ======================================
#
```

func_trans_save.in and func_trans_read.in are a pair of tests that check that the code can save a transmitted continuum then read it.

---

func_trans_read_lumi_scale.in

test read transmitted continuum in luminosity mode

```
title test read transmitted continuum in luminosity mode
#
# commands controlling continuum =========
table read "func_trans_save_lumi.trn" scale
# second, very faint SED to force luminosity mode
blackbody 50
luminosity 1
#
# commands for density & abundances =========
hden 3
#
# commands controlling geometry =========
radius 21
set dr 0
stop zone 1
#
# other commands for details =========
iterate
#
# commands controlling output =========
set save prefix "func_trans_read_lumi_scale"
save overview ".ovr"
save performance ".per"
save ionization last ".ion"
save continuum last ".con"
#
# this contains a large number of asserts that both tests use
init file "trans_lumi.dat"
#
# func_trans_read_lumi_scale.in
# class function
# ======================================
#
```

func_trans_lumi, func_trans_save_lumi, and func_trans_read_lumi_scale are a set of tests that check that the code can save a transmitted continuum in luminosity mode and then read it back in.

func_trans_lumi.in: this sim is directly illuminated by a BB at Rin = 1e21. Its predictions should be identical to func_trans_read_lumi_scale.in.

func_trans_save_lumi.in: this sim is directly illuminated by a BB at Rin = 1e20. It saves the transmitted continuum and has no monitors.

func_trans_read_lumi_scale.in: this sim is illiminated by the transmitted continuum at Rin = 1e21. Its predictions should be almost identical to func_trans_lumi.in. This tests that the transmitted continuum works correctly in luminosity mode and also that spherical dilution is handled correctly.

This sim must come after func_trans_save_lumi since it needs the save file generated by func_trans_save_lumi.

---

func_trans_read_scale.in

second of func_trans_save/func_trans_readread pair

```
title second of func_trans_save/func_trans_readread pair
# use the transmitted continuum produced by func_trans_save
#
# commands controlling continuum =========
# 10 continua scaled to 1/10 original should get same answer
table read "func_trans_save.trn" scale -1
table read "func_trans_save.trn" scale -1
table read "func_trans_save.trn" scale -1
table read "func_trans_save.trn" scale -1
table read "func_trans_save.trn" scale -1
table read "func_trans_save.trn" scale -1
table read "func_trans_save.trn" scale -1
table read "func_trans_save.trn" scale -1
table read "func_trans_save.trn" scale -1
table read "func_trans_save.trn" scale -1
#
# commands for density & abundances =========
hden 10
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
iterate
#
# commands controlling output =========
# this contains a large number of asserts used by both commands
init file "trans.dat"
save overview "func_trans_read_scale.ovr"
save performance "func_trans_read_scale.per"
save ionization last "func_trans_read_scale.ion"
# transmitted continuum should scale as specified
save last transmitted continuum "func_trans_read_scale.trn"
#
#
# func_trans_read_scale.in
# class function
# ========================================
#
```

func_trans_save.in and func_trans_read_scale.in are a pair of tests that check that the code can save a transmitted continuum then read it.

---

func_trans_save.in

first of func_trans_save/func_trans_read pair, save continuum

```
title first of func_trans_save/func_trans_read pair, save continuum
#
# commands controlling continuum =========
ionization parameter -1
table agn
#
# commands for density & abundances =========
```

```
hden 10
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
iterate
#
# commands controlling output =========
save overview "func_trans_save.ovr"
save performance "func_trans_save.per"
save ionization last "func_trans_save.ion"
save continuum last "func_trans_save.con"
# this continuum will be used by transread.in
save last transmitted continuum "func_trans_save.trn"
#
# this contains a large number of asserts that both tests use
init file "trans.dat"
#
# func_trans_save.in
# class function
# ======================================
#
```

func_trans_save, func_trans_read, func_trans_read_scale are a set of tests that check that the code can save a transmitted continuum then read it.

This sim must come before func_trans_read since it generates the save file needed by func_trans_read. Alphabetical order insures this.

---

func_trans_save_lumi.in

test save transmitted continuum in luminosity mode

```
title test save transmitted continuum in luminosity mode
#
# common commands
init file "func_trans_lumi.dat"
#
# commands controlling geometry =========
radius 20
#
# commands controlling output =========
set save prefix "func_trans_save_lumi"
save overview ".ovr"
save performance ".per"
save ionization last ".ion"
save continuum last ".con"
save transmitted continuum ".trn"
#
#
# func_trans_save_lumi.in
# class function
# ======================================
#
```

func_trans_lumi, func_trans_save_lumi, and func_trans_read_lumi_scale are a set of tests that check that the code can save a transmitted continuum in luminosity mode and then read it back in.

func_trans_lumi.in: this sim is directly illuminated by a BB at Rin = 1e21. Its predictions should be identical to func_trans_read_lumi_scale.in.

func_trans_save_lumi.in: this sim is directly illuminated by a BB at Rin = 1e20. It saves the transmitted continuum and has no monitors.

func_trans_read_lumi_scale.in: this sim is illiminated by the transmitted continuum at Rin = 1e21. Its predictions should be almost identical to func_trans_lumi.in. This tests that the transmitted continuum works correctly in luminosity mode and also that spherical dilution is handled correctly.

This sim must come before func_trans_read_lumi_scale since it generates the save file needed by func_trans_read_lumi_scale.

---

grains_hot.in

test temperature of gas and dust in high energy density environment

```
title test temperature of gas and dust in high energy density environment
#
# commands controlling continuum =========
table power law
# intensity of incident radiation field set by its energy density
energy density temp 550 K
#
# commands for density & abundances =========
hden 5.0
init "ism.ini"
# Orion grains and abundances
abundances orion
#
# commands controlling geometry =========
stop zone 1
set drmax 10
#
# other commands for details =========
#
# commands controlling output =========
normalize to "O 8" 18.9689A
save performance "grains_hot.per"
save overview "grains_hot.ovr" last
#
#
# grains_hot.in
# class limit
# ======================================
#
```

This tests the grains in an extreme condition - irradiation by an AGN near the illuminated face of the molecular torus. The gas is predominantly heated by the grain electron photo-ejection.

---

grains_hot_wd01.in

test temperature of gas and dust in high energy density environment

```
title test temperature of gas and dust in high energy density environment
#
# commands controlling continuum =========
table power law
energy density temp 550
#
# commands for density & abundances =========
hden 5.0
init "ism.ini"
```

```
abundances orion no grains
grains orion no qheat
#
# revert to WD01 treatment
no grain x-ray treatment
#
# commands controlling geometry =========
stop zone 1
set drmax 10
#
# other commands for details =========
#
# commands controlling output =========
normalize to "O 8" 18.9689A
save performance "grains_hot_wd01.per"
save overview "grains_hot_wd01.ovr" last
#
#
# grains_hot_wd01.in
# class limit
# ======================================
#
```

This tests the grains in an extreme condition - irradiation by an AGN near the illuminated face of the molecular torus. The gas is predominantly heated by the grains. The grain treatment has been reverted to Weingartner & Draine, 2001, which is NOT appropriate for these conditions. It is however a good test whether the old treatment is not broken....

---

grains_lte.in

check that grains equilibriate at correct temp in ste limit

```
title check that grains equilibriate at correct temp in ste limit
# this also tests that the code works when H He ionization is ZERO
#
# commands controlling continuum =========
black 3 lte
#
# commands for density & abundances =========
hden 5
eden 5
init file "hheonly.ini"
# need to normalize to some line, oxygen will provide some
element oxygen on
# ism grains with high dust to gas ratio
grain abund 1
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
iterate
cosmic rays background
database h2
#
# commands controlling output =========
save species "grains_lte.h" "H[:]" last densities
save species "grains_lte.h2" "H2[:]" last densities
normalize to "O 1" 63.1679m
save overview "grains_lte.ovr"
save performance "grains_lte.per"
save heating last "grains_lte.het"
save cooling last "grains_lte.col"
#
# grains_lte.in
```

```
# class limit
# ======================================
#
```

This test irradiates a set of grains with a true blackbody in strict thermodynamic equilibrium. We expect the grains (and everything else) to equilibriate at the blackbody temperature. The gas temperature is forced to the radiation temperature because the current molecule network (based on ISM approximations) does not go to LTE in the high-radiation density limit. The calculation asserts that all grain temperatures are very close to the radiation temperature.

---

grains_qheat.in

cool atomic ISM with Si grain quantum heating

```
title cool atomic ISM with Si grain quantum heating
#
# commands controlling continuum =========
table draine
extinguish 20
#
# commands for density & abundances =========
hden 0
# turns on grains with default abundance (log abundance ratio to ism = 0)
# and with quantum heating enabled by default
# (disabled with "no grains qheat" option)
grains 0. "silicate_ism_10.opc"
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
cosmic rays background
iterate
#
# commands controlling output =========
normalize to "c 2" 157.636m
print line faint -2
print line column
save overview "grains_qheat.ovr"
save performance "grains_qheat.per"
save grains temperature last "grains_qheat.qht"
save continuum "grains_qheat.con" units microns last
save two photon continuum "grains_qheat.2nu" units microns
save qheat last "grains_qheat.qhd"
#
#
# grains_qheat.in
# class limit
# ======================================
#
```

This sim produces dust emission with a Wein trail that is dominated by quantum heating emission.

---

grains_temp.in

test all grain species temperature

```
title test all grain species temperature
#
# commands controlling continuum =========
```

```
black 50000
ionization parameter -2
#
# commands for density & abundances =========
hden 3
grains "graphite_ism_01.opc"
grains "silicate_ism_01.opc"
grains "graphite_orion_01.opc"
grains "silicate_orion_01.opc"
grains "silicate_0m010.opc"
grains "silicate_0m100.opc"
grains "grey_ism_01.opc"
grains "silicate_1m000.opc"
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
iterate
constant temper 4
#
# commands controlling output =========
#
#
# grains_temp.in
# class limit
# ======================================
#
```

This turns on all the grain species that are included in the distribution. A model of an ionized layer is done and the monitors confirm the resulting grain temperatures.

---

grains_temp_all.in

test all grain species temperature

```
title test all grain species temperature
#
# commands controlling continuum =========
black 50000
ionization parameter -2
#
# commands for density & abundances =========
hden 3
# this turns on orion-style distributed grains
grains orion
# this turns on ism distributed grains
grains ism
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
constant temper 4
iterate
#
# commands controlling output =========
save overview "grains_temp_all.ovr"
save performance "grains_temp_all.per"
save dr "grains_temp_all.dr" last
save grain charge "grains_temp_all.grnchr" last
save grain temperature "grains_temp_all.grntem" last
save grain drift velocity "grains_temp_all.grndft" last
#
```

grains_temp_all.in # class limit # ===

This is a relatively quick test of grains. The Orion and ISM silicate and graphitic grains are turned on and their equilibrium temperature checked.

---

grains_xray.in

grains in a strong X-ray environment

```
title grains in a strong X-ray environment
#
# commands controlling continuum
table SED "grains_xray.sed"
ionization parameter = -2.000
#
# commands for density & abundances
hden = 3.000
grains ism
#
# commands controlling geometry
stop zone 1
#
# commands controlling output print and save commands
set save prefix "grains_xray"
save overview ".ovr"
save performance ".per"
#
```

This sim was added as a result of PR #523 https://gitlab.nublado.org/cloudy/cloudy/-/issues/523 The radiation field in grains_xray.sed has a very strong X-ray component, leading to lots of Auger and secondary electrons being emitted by the grain. This exposed a problem in the quantum heating treatment of these electrons.

---

grd_extreme_THiNhi.in

slow/grid_extreme highest density highest temperature

```
title slow/grid_extreme highest density highest temperature
set save prefix "grd_extreme_THiNhi"
#
element lithium off
element berylium off
element boron off
element limit -7 off
cosmic rays background linear 0.1266
cmb
iterate
#
# SED is 1e6 K BB with low energy density
blackbody 6
energy density 6
#
hden 18
stop zone 1
# set to constant small thickness
set dr -10
normalize to "Q(H)" 4861.32A
#
# the normalizing line is not defined on the emergent line stack
print lines emergent off
save performance no hash ".per"
```

```
#
# one of the four corners of grid_extreme,
# Figs 17&18 of 2013RMxAA..49..137F
```

---

grd_extreme_ThiNlo.in

slow/grid_extreme lowest density highest temperature

```
title slow/grid_extreme lowest density highest temperature
set save prefix "grd_extreme_ThiNlo"
#
element lithium off
element berylium off
element boron off
element limit -7 off
cosmic rays background linear 0.1266
cmb
iterate
#
# SED is 1e6 K BB with low energy density
blackbody 6
energy density 6
#
hden -8
stop zone 1
# set to constant small thickness
set dr -10
normalize to "Q(H)" 4861.32A
#
# the normalizing line is not defined on the emergent line stack
print lines emergent off
save performance no hash ".per"
#
# one of the four corners of grid_extreme,
# Figs 17&18 of 2013RMxAA..49..137F
```

---

grd_extreme_TloNhi.in

slow/grid_extreme highest density lowest temperature

```
title slow/grid_extreme highest density lowest temperature
set save prefix "grd_extreme_TloNhi"
#
element lithium off
element berylium off
element boron off
element limit -7 off
cosmic rays background linear 0.1266
cmb
iterate
#
# SED is 1e6 K BB with low energy density
blackbody 6
energy density 1
#
hden 18
stop zone 1
# set to constant small thickness
set dr -10
normalize to "Q(H)" 4861.32A
#
# the normalizing line is not defined on the emergent line stack
```

```
print lines emergent off
save performance no hash ".per"
#
# one of the four corners of grid_extreme,
# Figs 17&18 of 2013RMxAA..49..137F
```

---

grd_extreme_TloNlo.in

slow/grid_extreme lowest density lowest temperature

```
title slow/grid_extreme lowest density lowest temperature
set save prefix "grd_extreme_TloNlo"
#
element lithium off
element berylium off
element boron off
element limit -7 off
cosmic rays background linear 0.1266
cmb
iterate
#
# SED is 1e6 K BB with low energy density
blackbody 6
energy density 1
#
hden -8
stop zone 1
# set to constant small thickness
set dr -10
normalize to "Q(H)" 4861.32A
#
# the normalizing line is not defined on the emergent line stack
print lines emergent off
save performance no hash ".per"
# >>chng 25 05 30, <60 -> <70 include alldouble
#
# one of the four corners of grid_extreme,
# Figs 17&18 of 2013RMxAA..49..137F
```

---

grid_coronal.in

coronal equilibrium

```
title coronal equilibrium
#
# commands controlling continuum =========
coronal 4 vary
grid 1 9 0.25 sequential log
#
# commands for density & abundances =========
hden 0
#
# must include cosmic ray background since going below 1e4 K
cosmic ray background
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# commands controlling output =========
no blends
save grid "grid_coronal.grd" last no hash
```

```
save ages "grid_coronal.age" last no hash
save cooling "grid_coronal.col" last no hash
#
# grid_coronal.in
# class coronal
# ======================================
#
*********
```

This is a classical cooling function calculation - cosmic rays must be included for temperatures below 1e4 K to sustain the chemistry. This is a coronal (collisional) ionization calculation.

---

grid_coronal_grains.in

coronal equilibrium

```
title coronal equilibrium
#
# commands controlling continuum =========
coronal 4 vary
grid 1 9 0.25 sequential log
#
# commands for density & abundances =========
abundances ISM
grains PAH 3
hden 0
#
# must include cosmic ray background since going below 1e4 K
cosmic ray background
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# commands controlling output =========
no blends
save grid "grid_coronal_grains.grd" last no hash
save cooling "grid_coronal_grains.col" last no hash
#
# grid_coronal_grains.in
# class coronal
# ======================================
#
*********
```

this is a classical cooling function calculation - cosmic rays must be included for temperatures below 1e4 K to sustain chemistry. This is a coronal (collisional) ionization calculation. This case uses ISM abundances, depleted heavy elements, with grains

---

grid_coronal_primal.in

coronal equilibrium

```
title coronal equilibrium
#
# commands controlling continuum =========
coronal 4 vary
grid 1 9 0.25 sequential log
#
# commands for density & abundances =========
```

```
hden 0
abundances primordial
#
# must include cosmic ray background since going below 1e4 K
# make it 1e-4 of the default rate
cosmic ray background -4
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# commands controlling output =========
no blends
save grid "grid_coronal_primal.grd" last no hash
save cooling "grid_coronal_primal.col" last no hash
#
# grid_coronal_primal.in
# class coronal
# ======================================
#
*********
```

This is a classical cooling function calculation - cosmic rays must be included for temperatures below 1e4 K to sustain chemistry. This is a coronal (collisional) ionization calculation.

This version uses primordial abundances. A small CR rate has to be set for the low-T chemistry to work. The possibility of primordial cosmic rays is rays is mentioned by 2014A&A...570L...3T although thiey are not part of standard primrodial chemistry networks.

This is not a realistic model for several reasons. First, it uses the approximate small H2 model - the large model invoked with ATOM H2 is better but slower. Second, primordial chemistry is time dependent - the Universe is typically not old enough, at a given z, for the chemistry to have reached steady state. This is a time-steady calculation.

The purpose of the test is to demonstrate code behavior in the metal-free limit, over a wide range of temperature. Gas-phase light-element chemistry is exercised, but with the trace amount of cosmic rays.

---

grid_h2coronal.in

coronal equilibrium

```
title coronal equilibrium
#
# commands controlling continuum =========
coronal 4 vary
grid 1 9 0.25 log sequential
#
# commands for density & abundances =========
hden 0
# use all databases
database H2
database chianti levels max
database stout levels max
species "Fe+" levels=all
#
# must include cosmic ray background since going below 1e4 K
cosmic ray background
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# commands controlling output =========
no blends
```

```
save grid "grid_h2coronal.grd" last no hash
save cooling "grid_h2coronal.col" last no hash
#
# grid_h2coronal.in
# class coronal
# ======================================
#
*********
```

This is a classical cooling function calculation - cosmic rays must be included for temperatures below 1e4 K to sustain the chemistry. This is a coronal (collisional) ionization calculation.

It is a pair with grid_coronal - this uses complete species models, including all levels, while grid_coronal uses the default. There will be more cooling as a result, at a cost of more memory and greater execution time. This also serves as a test of the full Stout database

---

grid_h2coronal_primal.in

coronal equilibrium

```
title coronal equilibrium
set save prefix "grid_h2coronal_primal"
#
# commands controlling continuum =========
coronal 4 vary
grid 1 9 0.25 log sequential
#
# commands for density & abundances =========
hden 0
abundances primrodial
database H2
#
# must include cosmic ray background since going below 1e4 K
# make it 1e-4 of the default rate
cosmic ray background -4
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# commands controlling output =========
no blends
save grid ".grd" last no hash
save cooling ".col" last no hash
#
# grid_h2coronal_primal.in
# class coronal
# ======================================
#
*********
```

This is a classical cooling function calculation - cosmic rays must be included for temperatures below 1e4 K to sustain chemistry. This is a coronal (collisional) ionization calculation.

This version uses primordial abundances. A small CR rate has to be set for the low-T chemistry to work. The possibility of primordial cosmic rays is rays is mentioned by 2014A&A...570L...3T although thiey are not part of standard primrodial chemistry networks.

This is not a realistic model for several reasons. First, it uses the approximate small H2 model - the large model invoked with ATOM H2 is better but slower. Second, primordial chemistry is time dependent - the Universe is typically not old enough, at a given z, for the chemistry to have reached steady state. This is a time-steady calculation.

The purpose of the test is to demonstrate code behavior in the metal-free limit, over a wide range of temperature. Gas-phase light-element chemistry is exercised, but with the trace amount of cosmic rays.

---

h2_coll_t4.in

coronal equilibrium at 10^4 K

```
title coronal equilibrium at 10^4 K
#
# commands controlling continuum =========
coronal 4
#
# other commands for details =========
iterate
#
# commands controlling geometry =========
stop column density 15
#
# commands for density & abundances =========
hden 4
database H2
#
# commands controlling output =========
save performance "h2_coll_t4.per"
save overview "h2_coll_t4.ovr"
save continuum "h2_coll_t4.con" units angstroms
#
#
# h2_coll_t4.in
# class coronal
# ======================================
```

this tests conditions of collisional equilibrium at low densities

database h2 included to test results of large model Hden is 4 (coll_tx series is 10) to reproduce conditinos for major bug)

---

h2_cr.in

H2 with background cosmic ray ionization

```
title H2 with background cosmic ray ionization
#
# commands controlling continuum =========
# this is hot star SED
black 30000
intensity -5. range 0.4412 to 1 Ryd
# this will remove all ionizing radiation
extinguish 24 0
# background CR ionization rate of 2.5e-17 s^-1,
cosmic rays, background
#
# commands for density & abundances =========
hden 5
#
# commands controlling geometry =========
set dr 0
stop zone 5
stop temperature 400
#
# other commands for details =========
# failures should not occur
```

```
failures 1
database h2
iterate
# want clean test of CR physics so set constant kinetic temperature
constant temperature 500K
# must turn off line photoexcitation and Solomon process
# since we want to test cr heating and ionization
no induced processes
#
# commands controlling output =========
print column density
print ages
save performance "h2_cr.per"
save overview "h2_cr.ovr" last
save h2 lines "h2_cr.lin" last electronic all
save h2 rates "h2_cr.rat" last
save h2 column density "h2_cr.col" last
save dominant rates "h2_cr.h2" "H2" last
save chemistry rates "h2_cr.h2d" "H2" destruction
#
#
# h2_cr.in
# class limit
# ======================================
#
```

This test conditions of cosmic ray ionization. Solar abundances with no dust are assumed so this involves gas-phase chemistry alone. The Solomon process is disabled with the "no induced processes' command so H2 is mainly dissociated by cosmic rays. This forms a pair with h2_cr_grains, which does include grains.

---

h2_cr_grains.in

background cosmic ray ionization by suprathermal electrons only

```
title background cosmic ray ionization by suprathermal electrons only
#
# commands controlling continuum =========
# this is hot star continuum
black 30000
intensity -5. range 0.4412 to 1 Ryd
# this will remove all ionizing radiation
extinguish 24 0
# background CR ionization rate should be 2.5e-17 s^-1,
# Tielens & Hollenbach 1985; McKee AstroPH 9901370
cosmic rays, background
#
# commands for density & abundances =========
abundances ism
hden 5
#
# commands controlling geometry =========
set dr 0
stop zone 5
stop temperature 400
#
# other commands for details =========
set h2 grain formation thermal pump
database h2
iterate
constant temperature 500K
# must turn off line photoexcitation
# since we want to test cr heating and ionization
no induced processes
#
# commands controlling output =========
```

```
normalize to "H2 " 2.12125m
print column density
print ages
save performance "h2_cr_grains.per"
save overview "h2_cr_grains.ovr" last
save h2 lines "h2_cr_grains.lin" limit -10 last electronic all
save continuum units microns "h2_cr_grains.con" last
save h2 rates "h2_cr_grains.rat" last
save h2 column density "h2_cr_grains.col" last
save grains H2rates "h2_cr_grains.h2r" last
save dominant rates "h2_cr_grains.h2" "H2" last
save chemistry rates "h2_cr_grains.h2d" "H2" destruction
#
# h2_cr_grains.in
# class limit
# ======================================
#
```

This tests conditions of cosmic ray ionization and grain formation pumping. Solomon process is turned off with the "no induced processes" command so cosmic rays are the main dissociation process. This forms a pair with h2_cr which does not include grains, so relies only on gas-phase chemistry.

---

h2_hminus.in

H2 populations in H- dominated limit

```
title H2 populations in H- dominated limit
# this is one of a pair with h2_solomon.in
#
# commands controlling continuum =========
# this is hot star continuum
black 30000
intensity -5. range 0.4412 to 1 Ryd
# this will remove all ionizing radiation
extinguish 24 0
# background CR ionization rate should be 2.5e-17 s^-1,
# Tielens & Hollenbach 1985; McKee AstroPH 9901370
cosmic rays, background
#
# commands for density & abundances =========
# no grains in this sim so H2 forms by H- route
abundances ism no grains
hden 5
#
# commands controlling geometry =========
set dr 0
stop zone 5
stop temperature 400
#
# other commands for details =========
# default is Takahashi 2001 - test thermal distribution here
set h2 grain formation thermal pump
database h2
iterate
constant temperature 500K
#
# commands controlling output =========
print column density
print ages
save performance "h2_hminus.per"
save overview "h2_hminus.ovr" last
save h2 lines "h2_hminus.lin" last all
save h2 rates "h2_hminus.rat" last
save h2 column density "h2_hminus.col" last
save dominant rates "h2_hminus.h2" "H2" last
```

```
save chemistry rates "h2_hminus.h2d" "H2" destruction
#
# h2_hminus.in
# class limit
# ======================================
#
```

This tests large H2 model in limit of H- formation and Solomon destruction.

---

h2_pdr_leiden_f1.in

low density and flux model 1

```
title low density and flux model 1
set save prefix "h2_pdr_leiden_f1"
database H2 He collisions new
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 5
# this is to insure that no H-ionizing radiation strikes the cloud
extinguish 24
#
# commands for density & abundances =========
# hydrogen density
hden 3.
grains ism 1.16 no qheat
#
# commands controlling geometry =========
#
# other commands for details =========
# turn on the large H2 model
database h2
# turn down the number of convergence failures - there should be none
failures 3
# use leiden initialization file
init file="pdr_leiden.ini"
# This command defines the grain temperature to be a constant 20 Kelvin
constant grain temperature 20
# This sets the gas kinetic temperature to a constant 50 Kelvin
constant temperature 50 linear
#
# commands controlling output =========
# default normalization line is Hbeta, which is not produced by this gas
normalize to "c 2" 157.636m
print line faint -4
#
# saves
# check that all lines are found
table lines "LineList_PDR_H2.dat"
save performance ".per"
save overview ".ovr"
save fine optical depths last no hash ".fopt" range 1150 1300 units Angstroms 1
save save emitted continuum ".econ" range 1150 1300 units angstroms
save line emissivity ".ems"
H2 2.12125m
CO 650.074m
C 2 157.636m
O 1 63.1679m
Si 2 34.8046m
end of lines
save leiden lines ".lin"
save leiden ".lei"
```

```
save dr ".dr"
save molecules ".mol"
save grain physical conditions ".grn"
save overview ".ovr"
save H2 lines ".h2lin" all
save H2 column density ".h2col"
save H2 populations matrix zone ".pop"
save H2 rates ".rat"
save dominant rates ".h2" "H2"
save chemistry rates ".h2d" "H2" destruction
#
#
# h2_pdr_leiden_f1.in
# class pdr
# ======================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187

---

h2_solomon.in

H2 populations in solomon dominated limit

```
title H2 populations in solomon dominated limit
# this is a pair with h2_hminus
#
# commands controlling continuum =========
# this is hot star continuum
black 30000
intensity -5. range 0.4412 to 1 Ryd
# this will remove all ionizing radiation
extinguish 24 0
# background CR ionization rate should be 2.5e-17 s^-1,
# Tielens & Hollenbach 1985; McKee AstroPH 9901370
cosmic rays, background
#
# commands for density & abundances =========
abundances ism
hden 5
#
# commands controlling geometry =========
set dr 0
stop zone 5
stop temperature 400
#
# other commands for details =========
# default is Takahashi 2001 - test thermal distribution here
set h2 grain formation thermal pump
database h2
iterate
constant temperature 500K
#
# commands controlling output =========
# don't print so many lines
print line faint 10
print line column
print line sort wavelength
print column density
print ages
save performance "h2_solomon.per"
save overview "h2_solomon.ovr" last
save h2 lines "h2_solomon.lin" limit -10 last all electronic all
save h2 rates "h2_solomon.rat" last
save h2 column density "h2_solomon.col" last
save continuum units microns "h2_solomon.con" last
```

```
save dominant rates "h2_solomon.h2" "H2" last
save chemistry rates "h2_solomon.h2d" "H2" destruction
#
# h2_solomon.in
# class limit
# ======================================
#
```

This test H2 in case of grain formation and solomon destruction

---

h2_t2000.in

test large H2 molecule in shock-like conditions

```
title test large H2 molecule in shock-like conditions
#
# commands controlling continuum =========
# there is a continuum but it is unimportant
# first continuum is FIR hot grain continuum produced in
# unmodeled HII Region
black 30000
intensity -5 range 0.4412 to 1 Ryd
# this will remove all ionizing radiation
extinguish 24 0
# must provide source of ionization for chemistry
cosmic rays, background
#
# commands for density & abundances =========
hden 6
grains ism, abundance log 0.16 single
init file="ism.ini"
abundances he= -1.01 c= -3.52 n=-8 o=-3.30 ne=-8 mg=-5.89
continue si= -6.10 s= -5.10 cl=-7 ar=-8 fe= -6.60
#
# commands controlling geometry =========
stop zone 10
# force zone thickess to 1 cm
set dr 0
# need to lower stop temperature since gas is cooler than 4000K
stop temperature 3
#
# other commands for details =========
failures 2
database h2
constant temperature 2000
iterate
# this stop Lymnan line excitation of H, which is then photoionized
# by Balmer continuum
Database H-like Lyman pumping off
#
# commands controlling output =========
normalize to "H2 " 2.12125m
#
save performance "h2_t2000.per"
save dominant rates "h2_t2000.oh" "OH" last
save dominant rates "h2_t2000.ohp" "OH+" last
save dominant rates "h2_t2000.h2" "H2" last
save pdr "h2_t2000.pdr"
save h2 rates "h2_t2000.rat"
save h2 column density "h2_t2000.col"
save h2 lines "h2_t2000.lin" all last
save h2 populations "h2_t2000.pop" all last
save chemistry rates "h2_t2000.h2d" "H2" destruction
save raw continuum "h2_t2000.raw"
save continuum "h2_t2000.con"
```

```
save overview "h2_t2000.ovr"
save species column densities "h2_t2000.scol" all
save species departures "h2_t2000.sdep" "H2O[:]"
save species densities "h2_t2000.spop" all
save species energies "h2_t2000.senr" "H2O[:]"
save species column densities "h2_t2000.scolH2O" "H2O[:]"
save species densities "h2_t2000.spopH2O" "H2O[:]"
#
# h2_t2000.in
# class limit
# ======================================
```

This is a collisionally dominated H2 simulation. The temperature has been fixed at 2000K and the large molecule turned on. The calculation checks the returned value of the ortho to para densities. Cosmic rays and the incident continuum have little effect, the density is high, so the populations should be close to LTE.

---

h2_t500.in

```
set h2 continuum dissociation Stancil
```

test large H2 molecule in PDR-like conditions

```
title test large H2 molecule in PDR-like conditions
#
# commands controlling continuum =========
# first continuum is FIR hot grain continuum produced in
# unmodeled HII Region
blackbody, t = 75 K
intensity -2.7 (total)
# this is hot star continuum
black 30000
intensity -5 range 0.4412 to 1 Ryd
# this will remove all ionizing radiation
extinguish 24 0
#
# commands for density & abundances =========
hden 6
grains ism, abundance log 0.16 single, no qheat
init file="ism.ini"
abundances he= -1.01 c= -3.52 n=-8 o=-3.30 ne=-8 mg=-5.89
continue si= -6.10 s= -5.10 cl=-7 ar=-8 fe= -6.60
turbulence 2.7 km/sec
#
# commands controlling geometry =========
stop zone 10
# force zone thickess to 1 cm
sphere
set dr 0
# stop when gas is fully neutral
stop efrac -10
# stop when gas is cold
stop temperature 10 linear
#
# other commands for details =========
failures 2
database h2
constant temperature 500
iterate
Database H-like Lyman pumping off
cosmic rays background
#
# commands controlling output =========
normalize to "CO " 866.727m
# uv lines are strongly pumped by stellar continuum, break out contribution
```

```
print line pump
print line optical depths
print line faint -2
print ages
#
save performance "h2_t500.per"
save cooling "h2_t500.col"
save pdr "h2_t500.pdr"
save H2 rates "h2_t500.rat"
save H2 lines "h2_t500.lin" all
save H2 column density "h2_t500.h2col"
save H2 populations "h2_t500.pop"
save H2 levels "h2_t500.lev"
save raw continuum "h2_t500.raw"
save continuum "h2_t500.con"
save overview "h2_t500.ovr"
save dominant rates "h2_t500.h2" "H2"
save chemistry rates "h2_t500.h2d" "H2" destruction
#
# h2_t500.in
# class limit
# ======================================
```

This is a dense molecular gas with background cosmic rays and the incident radiation field set to a small value. The lower levels are in LTE.

---

h_otsopen.in

test ots, inward fractions for pure hydrogen, open geo, filling factor

```
title test ots, inward fractions for pure hydrogen, open geo, filling factor
#
# commands controlling continuum =========
ionization -2
blackbody 40000
#
# commands for density & abundances =========
hden 5
init file "honly.ini"
#
# commands controlling geometry =========
constant temper 7500
filling factor 0.01
#
# other commands for details =========
# must iterate to get inward line fractions, that are asserted below
iterate
diffuse ots
# not iterating does not affect the solution
no level2
no induced processes (OK)
#
# commands controlling output =========
print line inward
save performance "h_otsopen.per"
save overview "h_otsopen.ovr" last
save dr "h_otsopen.dr" last
save continuum "h_otsopen.con" last units angstrom
#
# this is an open geometry, so do not expect H atom to exactly be case B
# due to Lyman line leakage. we iterated, so have a good estimate of
# inward and outward fractions, which we test
# h_otsopen.in
# class limit
```

```
# ======================================
#
```

This tests the total emission from a hydrogen Stromgren sphere using the OTS approximation. The conservation of the total number of ionizing photons, and the emitted spectrum, are all checked.

---

h_otspp.in

plane parallel conservation and hydrogenic emission for pure hydrogen

```
title plane parallel conservation and hydrogenic emission for pure hydrogen
#
# commands controlling continuum =========
ionization -2
blackbody 40000
#
# commands for density & abundances =========
hden 5
init file "honly.ini"
#
# commands controlling geometry =========
sphere static (OK)
#
# other commands for details =========
constant temper 7500
no level2
no induced processes (OK)
# needed to prevent 2s / Bal from becoming optically thick
turbulence 20 km/s
diffuse ots
database h-like levels resolved 10
#
# commands controlling output =========
save performance "h_otspp.per"
save overview "h_otspp.ovr"
save dr "h_otspp.dr"
#
# h_otspp.in
# class limit
# ======================================
#
```

This tests the total emission from a plane parallel pure hydrogen Stromgren sphere using the OTS approximation. The conservation of the total number of ionizing photons, and the emitted spectrum, are all checked.

---

h_otssp.in

spherical conservation and hydrogenic emission for pure hydrogen

```
title spherical conservation and hydrogenic emission for pure hydrogen
#
# commands controlling continuum =========
ionization -2
blackbody 40000
#
# commands for density & abundances =========
hden 5
init file "honly.ini"
#
# commands controlling geometry =========
radius 13
```

```
# not iterating does not affect the solution
sphere static (OK)
#
# other commands for details =========
constant temper 7500
diffuse ots
no level2
no induced processes (OK)
#
# commands controlling output =========
save performance "h_otssp.per"
save overview "h_otssp.ovr"
save dr "h_otssp.dr"
#
# h_otssp.in
# class limit
# ======================================
#
```

This tests the total emission from a spherical pure hydrogen Stromgren sphere using the OTS approximation. The conservation of the total number of ionizing photons, and the emitted spectrum, are all checked.

---

h_outopen.in

test open geometry

```
title test open geometry
#
# commands controlling continuum =========
ionization -2
blackbody 40000
#
# commands for density & abundances =========
hden 0
init file "honly.ini"
#
# commands controlling geometry =========
filling 0.01
#
# other commands for details =========
diffuse outward
iterate
database h-like levels resolved 15
no level2
no induced processes (OK)
constant temper 4
#
# commands controlling output =========
# normally will not print out inward parts of lines
print line inward
save performance "h_outopen.per"
save overview "h_outopen.ovr" last
save dr "h_outopen.dr" last
#
# this is an open geometry, so do not expect H atom to exactly be case B
# due to Lyman line leakage. we iterated, so have a good estimate of
# inward and outward fractions, which we test
# h_outopen.in
# class limit
# ======================================
#
```

This tests the total emission from an open geometry, hydrogen Stromgren sphere, using the outward only approximation. The conservation of the total number of ionizing photons, and the emitted spectrum, are all checked.

---

h_outpp.in

plane parallel H-only, close, test hydrogenic emission

```
title plane parallel H-only, close, test hydrogenic emission
#
# commands controlling continuum =========
ionization -2
blackbody 40000
#
# commands for density & abundances =========
# the hydrogen density
hden 5
# an ini file that will include H-only
init file "honly.ini"
#
# commands controlling geometry =========
# need this to prevent lyman lines from escaping
sphere static (OK)
#
# other commands for details =========
# prevent continuum pumping of lyman lines
no induced processes (OK)
# must include this to keep Ha optically thin
turbulence 20 km/s
# this is the approximation we are testing
diffuse outward
# force a constant temperature, then give stopping criteria
# if stop were not present model would go to limiting number of zones
constant temper 7500
# increase number of levels to get full emission
database h-like levels resolved 20
#
# commands controlling output =========
# need to turn this on so that continua at various energies will
# be included in the emission line list
# normalize results to perfect case b - our predictions should
# be close to this
# the output and asserts
save performance "h_outpp.per"
save overview "h_outpp.ovr"
save dr "h_outpp.dr"
#
# energies dominated by two photon emission not included since very
# sensitive to Lya transport
# h_outpp.in
# class limit
# ======================================
#
```

This tests the total emission from a plane parallel pure hydrogen Stromgren sphere using the outward only approximation. The conservation of the total number of ionizing photons, and the emitted spectrum, are all checked.

---

h_outsp.in

spherical conservation and hydrogenic emission for pure hydrogen

```
title spherical conservation and hydrogenic emission for pure hydrogen
#
# commands controlling continuum =========
ionization -2
blackbody 40000
```

```
#
# commands for density & abundances =========
hden 5
init file "honly.ini"
#
# commands controlling geometry =========
radius 13
# not iterating does not affect the solution
sphere static (OK)
#
# other commands for details =========
constant temper 7500
no level2
database h-like levels resolved 20
no induced processes (OK)
diffuse outward
#
# commands controlling output =========
save performance "h_outsp.per"
save overview "h_outsp.ovr"
save dr "h_outsp.dr"
#
# energies dominated by two photon emission not included since very
# sensitive to Lya transport
# h_outsp.in
# class limit
# ======================================
#
```

This tests the total emission from a spherical pure hydrogen Stromgren sphere using the outward only approximation. The conservation of the total number of ionizing photons, and the emitted spectrum, are all checked.

---

h_t4_conemis.in

continuous emission from H atom

```
title continuous emission from H atom
#
# commands controlling continuum =========
# use laser so that stellar continuum is not in predicted continuum
laser 2
ionization -1
#
# commands for density & abundances =========
# high density to suppress two-photon emission
hden 8
init "honly.ini"
#
# commands controlling geometry =========
# this thisckness is the inverse square of the density, so the
# total emission from the computed slab will in effect have the
# square of the density removed, so predictions will be j pi j / n_e n_p
stop thickness -16
#
# other commands for details =========
# include a large number of levels to capture IR emission
# increase default resolution stored in continuum_mesh.ini
set continuum resolution 0.1
iterate
constant temperature 4
#
# commands controlling output =========
print lines column
save overview "h_t4_conemis.ovr"
save performance "h_t4_conemis.per"
```

```
save continuum "h_t4_conemis.con" last no title units microns
#
# h_t4_conemis.in
# class limit
# ======================================
#
```

This tests the continuous emission from the model H atom. The gas temperature is 10000 K and the continuous emissivity is asserted for a range of wavelengths.

This was used to generate the plot in Hazy 2 comparing the emission from a pure hydrogen plasma with those of Ferland 1980.

>>refer HI emission Ferland, G. J. 1980, PASP, 92, 596

---

h_t4_conemis_lon.in

low-den continuous HI emission with 2-nu important

```
title low-den continuous HI emission with 2-nu important
#
# commands controlling continuum =========
laser 2
ionization -1
#
# commands for density & abundances =========
hden 0
init "honly.ini"
#
# commands controlling geometry =========
stop thickness 0
#
# other commands for details =========
# increase default resolution stored in continuum_mesh.ini
set continuum resolution 0.1
case b
iterate
constant temperature 4
#
# commands controlling output =========
print lines column
save overview "h_t4_conemis_lon.ovr"
save performance "h_t4_conemis_lon.per"
save continuum "h_t4_conemis_lon.con" last units microns
save two photon continuum "h_t4_conemis_lon.2nu" last rydbergs
#
# h_t4_conemis_lon.in
# class limit
# ======================================
#
```

This is a mate to hatomt10.in except that the density is low enough for two-photon emission to be very imporant in the optical and uv.

---

h_t4_conemis_thick.in

H I continuous emissivity, used for plot in hazy

```
title H I continuous emissivity, used for plot in hazy
#
```

```
# commands controlling continuum =========
black 5
ionization parameter -2
#
# commands for density & abundances =========
# high density to suppress two-photon emission
hden 7
# turn off all elements, except for hydrogen, so that
# we really test hydrogen emission
init file= "honly.ini"
#
# commands controlling geometry =========
# this is necessary to stop model at H ionization front
# constant temperature models will go on to infinity without this
stop efrac -0.8
#
# other commands for details =========
# increase continuum resolution by factor of ten
set continuum resolution 0.1
# line fluorescense would be very important with above turbulence,
# turn it off
no induced processes
# need large atom to get the many Rydgerg levels in the infrared
# atom h-like levels resolved 10
# what full outward flux so use spherical geometry
sphere
constant temperature 4
#
# commands controlling output =========
# results will be relative to interplated Hummer&Storey Hbeta
# this tests hydrogen atom too
# output the predicted continuum
save overview "h_t4_conemis_thick.ovr"
save performance "h_t4_conemis_thick.per"
save emitted continuum last iteration "h_t4_conemis_thick.con" units micron
save dr last "h_t4_conemis_thick.dr"
#
# h_t4_conemis_thick.in
# class limit
# ======================================
#
```

This checks that the predicted hydrogen continuum is in good agreement with exact results in the optically thin nebular limit.

Checks:
- This output was used to generate figure h_t4_conemis_thick in Part I of HAZY.
- Continuum relative to Hbeta should agree with Ferland (1980) filter averaged results.
- Hbeta should agree with Case B predictions, and Q(H) 4861.

---

heatomt10.in

continuous emission from HeI

```
title continuous emission from HeI
#
# commands controlling continuum =========
laser 1.9 ryd
ionization -1
#
# commands for density & abundances =========
# need high density to supress two-photon emission
hden 10
```

```
# force high density for electrons, He+ density will be the same
set eden 12
# set He/H ratio to 100, He and elec will have same density
element abundance helium 2
init "hheonly.ini"
#
# commands controlling geometry =========
# this thickness will get unit emission when combined with above densities
stop thickness -24
#
# other commands for details =========
iterate
constant temperature 4
#
# commands controlling output =========
#
set continuum resolution 0.1
set nFnu diffuse outward, diffuse inward
print line faint 1
print line column
save overview "heatomt10.ovr"
save performance "heatomt10.per"
save continuum "heatomt10.con" last no title units microns
save diffuse continuum "heatomt10.dif" last no title units microns
#
# heatomt10.in
# class limit
# ======================================
#
```

This tests continuous emission from the He I atom. The laser is used so that the incident continuum is not included in the total emission.

---

heatomt10lon.in

test low-den continuous emission from H atom, 2-nu is important

```
title test low-den continuous emission from H atom, 2-nu is important
#
# commands controlling continuum =========
laser 2
ionization -1
#
# commands for density & abundances =========
hden -8
element helium abundance log 3
set eden -5
init "hheonly.ini"
#
# commands controlling geometry =========
stop thickness log 10
#
# other commands for details =========
no scattering opacity
# force all helium to be in He+
element helium ionization -4 0 -4
case b
# increase default resolution stored in continuum_mesh.ini
set continuum resolution 0.1
iterate
constant temperature 4
#
# commands controlling output =========
normalize to "Blnd" 4472.76A vacuum
print lines column
```

```
print lines column
save overview "heatomt10lon.ovr"
save performance "heatomt10lon.per"
save continuum "heatomt10lon.con" last units microns
save diffuse continuum "heatomt10lon.dif" last units microns
save two photon continuum "heatomt10lon.2nu" last
#
# heatomt10lon.in
# class limit
# ======================================
#
```

This is a mate to hatomt10.in except that everything is He at low density

---

heiont10.in

continuous emission from HeII

```
title continuous emission from HeII
#
# commands controlling continuum =========
laser 5 ryd
ionization 1
#
# commands for density & abundances =========
hden 8
set eden 10
element abundance helium 2
init "hheonly.ini"
#
# commands controlling geometry =========
stop thickness -20
#
# other commands for details =========
constant temperature 4
iterate
# increase continuum resolution by factor of ten
set continuum resolution 0.1
set nFnu diffuse outward, diffuse inward
#
# commands controlling output =========
print line faint 1
print line column
save overview "heiont10.ovr"
save performance "heiont10.per"
save continuum "heiont10.con" last no title units microns
#
# heiont10.in
# class limit
# ======================================
#
```

This tests the He II continuous emission. The helium abundance is very large so that He II overwhelms other emission sources. The resolution of the continuum mesh is increased so that we get a better representation of the continuous emission.

---

helike_ar.in

He-like argon emission

```
title He-like argon emission
#
```

```
# commands controlling continuum =========
laser 600
ionization -1
#
# commands for density & abundances =========
hden 7
# include lots of the element we are testing and set the ionization
# to be dominated by the correct ion stage
element argon abundance -2
element argon ionization -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 0 -5
init file "ism.ini"
element helium off
element carbon off
element nitrogen off
element oxygen off
element neon off
element magnesium off
element silicon off
element sulphur off
element chlorine off
element iron off
#
# commands controlling geometry =========
set dr -12
stop zone 1
#
# other commands for details =========
database he-like resolved levels 10
database he-like collapsed levels 20
constant temper 5
iterate
#
# commands controlling output =========
print he-like departure argon
print line faint -5
save overview "helike_ar.ovr"
save performance "helike_ar.per"
# This is Lyman alpha
normalize to "Ar17" 3.94907A
#
# 3.994A is 2^3S to ground
# Totl is 2^3P to ground
# 3.365A is 3^1P to ground
# 21.54A is 3^3P to 2^3S
# 22.24A is 3^3D to 2^3P
#
# helike_ar.in
# class limit
# ======================================
#
```

test He-like emission for argon

---

helike_c.in

he-like carbon emission

```
title he-like carbon emission
#
# commands controlling continuum =========
laser 50
ionization -1
#
# commands for density & abundances =========
hden 7
```

```
# include lots of the element we are testing and set the ionization
# to be dominated by the correct ion stage
element carbon abundance -2
element carbon ionization -5 -5 -5 -5 -5 0 -5
init file "ism.ini"
element helium off
element nitrogen off
element oxygen off
element neon off
element magnesium off
element silicon off
element sulphur off
element chlorine off
element argon off
element iron off
#
# commands controlling geometry =========
set dr -12
stop zone 1
#
# other commands for details =========
database he-like resolved levels 10
database he-like collapsed levels 20
constant temper 5
iterate
#
# commands controlling output =========
print he-like departure carbon
print line faint -2
save overview "helike_c.ovr"
save performance "helike_c.per"
# This is Lyman alpha
normalize to "C 5" 40.2678A
#
#
# helike_c.in
# class limit
# ======================================
#
```

test he-like carbon emission

---

helike_co.in

He-like cobalt emission

```
title He-like cobalt emission
database he-like resolved levels 10
database he-like collapsed levels 20
print he-like departure cobalt
constant temper 5
iterate
hden 7
set dr -12
init file "ism.ini"
# must turn on since ism.ini turned it off
element cobalt on
# then set abundance and ionization after turning it on
element cobalt abundance -2
element cobalt ionization -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5
-5 0 -5
# now turn lots of elements off to save time
element helium off
element carbon off
element nitrogen off
```

```
element oxygen off
element neon off
element magnesium off
element silicon off
element sulphur off
element chlorine off
element argon off
element iron off
laser 1300
ionization -1
stop zone 1
print line faint -2
save overview "helike_co.ovr"
save performance "helike_co.per"
#
# helike_co.in
# class limit
# ========================================
#
```

test emission of He-like Co

---

helike_cu.in

He-like copper emission

```
title He-like copper emission
database he-like resolved levels 10
database he-like collapsed levels 20
print he-like departure copper
constant temper 5
iterate
hden 7
set dr -12
init file "ism.ini"
# must turn on since ism.ini turned it off
element copper on
# then set abundance and ionization after turning it on
element copper abundance -2
element copper ionization -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5
-5 -5 -5 0 -5
# now turn lots of elements off to save time
element helium off
element carbon off
element nitrogen off
element oxygen off
element neon off
element magnesium off
element silicon off
element sulphur off
element chlorine off
element argon off
element iron off
laser 1300
ionization -1
stop zone 1
print line faint -2
save overview "helike_cu.ovr"
save performance "helike_cu.per"
#
# helike_cu.in
# class limit
# ========================================
#
```

test emission of He-like Cu

---

helike_fe.in

he-like iron emission

```
title he-like iron emission
#
# commands controlling continuum =========
laser 1300
ionization -1
#
# commands for density & abundances =========
hden 7
set dr -12
# include lots of the element we are testing and set the ionization
# to be dominated by the correct ion stage
element iron abundance -2
element iron ionization -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 0
-5
init file "ism.ini"
element helium off
element carbon off
element nitrogen off
element oxygen off
element neon off
element magnesium off
element silicon off
element sulphur off
element chlorine off
element argon off
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
database he-like resolved levels 10
database he-like collapsed levels 20
constant temper 5
iterate
#
# commands controlling output =========
print line faint -2
print he-like departure iron
save overview "helike_fe.ovr"
save performance "helike_fe.per"
# This is Lyman alpha
normalize to "Fe25" 1.8504A
#
#
# helike_fe.in
# class limit
# ======================================
#
```

check He-like emission for iron

---

helike_mg.in

he-like magnesium emission

```
title he-like magnesium emission
#
# commands controlling continuum =========
laser 250
ionization -1
#
# commands for density & abundances =========
hden 7
set dr -12
element magnesium abundance -2
element magnesium ionization -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 0 -5
init file "ism.ini"
element helium off
element carbon off
element nitrogen off
element oxygen off
element neon off
element silicon off
element sulphur off
element chlorine off
element argon off
element iron off
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
database he-like resolved levels 10
database he-like collapsed levels 20
constant temper 5
iterate
#
# commands controlling output =========
print he-like departure magnesium
print line faint -2
save overview "helike_mg.ovr"
save performance "helike_mg.per"
# This is Lyman alpha
normalize to "Mg11" 9.16875A
#
#
# helike_mg.in
# class limit
# ======================================
#
```

test He-like Mg emission

---

helike_n.in

He-like nitrogen emission

```
title He-like nitrogen emission
#
# commands controlling continuum =========
laser 75
ionization -1
#
# commands for density & abundances =========
hden 7
element nitrogen abundance -2
element nitrogen ionization -5 -5 -5 -5 -5 -5 0 -5
init file "ism.ini"
element helium off
```

```
element carbon off
element oxygen off
element neon off
element magnesium off
element silicon off
element sulphur off
element chlorine off
element argon off
element iron off
#
# commands controlling geometry =========
stop zone 1
set dr -12
#
# other commands for details =========
database he-like resolved levels 10
database he-like collapsed levels 20
constant temper 5
iterate
#
# commands controlling output =========
print he-like departure nitrogen
print line faint -2
save overview "helike_n.ovr"
save performance "helike_n.per"
# This is Lyman alpha
normalize to "N 6" 28.7870A
#
# helike_n.in
# class limit
# ======================================
#
```

test He-like emission for N

---

helike_ne.in

he-like neon emission

```
title he-like neon emission
#
# commands controlling continuum =========
laser 170
ionization -1
#
# commands for density & abundances =========
hden 7
# include lots of the element we are testing and set the ionization
# to be dominated by the correct ion stage
element neon abundance -2
element neon ionization -5 -5 -5 -5 -5 -5 -5 -5 -5 0 -5
init file "ism.ini"
element helium off
element carbon off
element nitrogen off
element oxygen off
element magnesium off
element silicon off
element sulphur off
element chlorine off
element argon off
element iron off
#
# commands controlling geometry =========
stop zone 1
```

```
set dr -12
#
# other commands for details =========
database he-like resolved levels 10
database he-like collapsed levels 20
constant temper 5
iterate
#
# commands controlling output =========
print he-like departure neon
print line faint -2
save overview "helike_ne.ovr"
save performance "helike_ne.per"
# This is Lyman alpha
normalize to "Ne 9" 13.4471A
#
#
# helike_ne.in
# class limit
# ======================================
#
```

test He-like emission for oxygen

---

helike_ni.in

he-like nickel emission

```
title he-like nickel emission
database he-like resolved levels 10
database he-like collapsed levels 20
print he-like departure nickel
constant temper 5
iterate
hden 7
set dr -12
init file "ism.ini"
# must turn on since ism.ini turned it off
element nickel on
# then set abundance and ionization after turning it on
element nickel abundance -2
element nickel ionization -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5
-5 -5 0 -5
# now turn lots of elements off to save time
element helium off
element carbon off
element nitrogen off
element oxygen off
element neon off
element magnesium off
element silicon off
element sulphur off
element chlorine off
element argon off
element iron off
laser 1300
ionization -1
stop zone 1
print line faint -2
save overview "helike_ni.ovr"
save performance "helike_ni.per"
#
# helike_ni.in
# class limit
```

```
# ======================================
#
```

Test He-like Ni emission.

---

helike_o.in

he-like oxygen ion vs. Bautista & Kallman 2000 Table 1, column 3

```
title he-like oxygen ion vs. Bautista & Kallman 2000 Table 1, column 3
#
# commands controlling continuum =========
laser 100
ionization -1
#
# commands for density & abundances =========
hden 7
# include lots of the element we are testing and set the ionization
# to be dominated by the correct ion stage
element oxygen abundance -2
element oxygen ionization -5 -5 -5 -5 -5 -5 -5 0 -5
init file "ism.ini"
element helium off
element carbon off
element nitrogen off
element neon off
element magnesium off
element silicon off
element sulphur off
element chlorine off
element argon off
element iron off
#
# commands controlling geometry =========
stop zone 1
set dr -12
#
# other commands for details =========
database he-like resolved levels 10
database he-like collapsed levels 20
constant temper 5
iterate
#
# commands controlling output =========
print he-like departure oxygen
print line sort wavelength
print line faint -5
save overview "helike_o.ovr"
save performance "helike_o.per"
save continuum "helike_o.con" units Angstroms
normalize to "o 7" 21.6020A
#
# helike_o.in
# class limit
# ======================================
#
```

test He-like emission for oxygen

---

helike_si.in

He-like silicon emission

```
title He-like silicon emission
#
# commands controlling continuum =========
laser 350
ionization -1
#
# commands for density & abundances =========
hden 7
# include lots of the element we are testing and set the ionization
# to be dominated by the correct ion stage
element silicon abundance -2
element silicon ionization -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 0 -5
init file "ism.ini"
element helium off
element carbon off
element nitrogen off
element oxygen off
element neon off
element magnesium off
element sulphur off
element chlorine off
element argon off
element iron off
#
# commands controlling geometry =========
stop zone 1
set dr -12
#
# other commands for details =========
database he-like resolved levels 10
database he-like collapsed levels 20
constant temper 5
iterate
#
# commands controlling output =========
print he-like departure silicon
print line faint -2
save overview "helike_si.ovr"
save performance "helike_si.per"
# This is Lyman alpha
normalize to "Si13" 6.64803A
#
#
# helike_si.in
# class limit
#
```

test He-like emission for silicon

---

helike_zn.in

He-like zinc emission

```
title He-like zinc emission
database he-like resolved levels 10
database he-like collapsed levels 20
print he-like departure zinc
constant temper 5
iterate
hden 7
set dr -12
init file "ism.ini"
# must turn on since ism.ini turned it off
element zinc on
```

```
# then set abundance and ionization after turning it on
element zinc abundance -2
element zinc ionization -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5 -5
-5 -5 -5 0 -5
# now turn lots of elements off to save time
element helium off
element carbon off
element nitrogen off
element oxygen off
element neon off
element magnesium off
element silicon off
element sulphur off
element chlorine off
element argon off
element iron off
laser 1300
ionization -1
stop zone 1
print line faint -2
save overview "helike_zn.ovr"
save performance "helike_zn.per"
#
# helike_zn.in
# class limit
# ======================================
#
```

test emission for He-like Zn

---

hhe_otspp.in

plane parallel conservation and H-like emission for H, He

```
title plane parallel conservation and H-like emission for H, He
#
# commands controlling continuum =========
ionization -2
blackbody 40000
#
# commands for density & abundances =========
hden 5
init file "hheonly.ini"
#
# commands controlling geometry =========
# expanding sphere to stop Lya from destroying HeI 23S
sphere
#
# other commands for details =========
diffuse ots
database h-like element hydrogen levels resolved 10
# need to iterate since we will assert helium triplet lines
# that depend on having stable solution
iterate
constant temper 7500
no induced processes (OK)
#
# commands controlling output =========
save performance "hhe_otspp.per"
save overview "hhe_otspp.ovr" last
save dr "hhe_otspp.dr" last
#
# helium lines
# hhe_otspp.in
# class limit
```

```
# ======================================
#
```

This tests the total emission from a spherical pure H + He Stromgren sphere using the outward only approximation. The conservation of the total number of ionizing photons, and the emitted spectrum, are all checked.

---

hhe_otssp.in

spherical conservation and H-like emission for H and He

```
title spherical conservation and H-like emission for H and He
#
# commands controlling continuum =========
blackbody 40000
ionization -2
#
# commands for density & abundances =========
hden 5
init file "hheonly.ini"
#
# commands controlling geometry =========
diffuse ots
database h-like levels resolved 10
radius 13
sphere static
#
# other commands for details =========
constant temper 7500
iterate
no level2
no induced processes (OK)
#
# commands controlling output =========
save performance "hhe_otssp.per"
save overview "hhe_otssp.ovr" last
save dr "hhe_otssp.dr" last
#
# helium lines
# hhe_otssp.in
# class limit
# ======================================
#
```

This tests the total emission from a spherical pure H + He-like Stromgren sphere using the outward only approximation. The conservation of the total number of ionizing photons, and the emitted spectrum, are all checked. The geometry is plane paralel.

---

hhe_outpp.in

plane parallel conservation emission for H, He gas

```
title plane parallel conservation emission for H, He gas
#
# commands controlling continuum =========
blackbody 40000
ionization -2
#
# commands for density & abundances =========
hden 5
init file "hheonly.ini"
```

```
#
# commands controlling geometry =========
# open sphere to stop Lya from destroying HeI 23S
sphere
#
# other commands for details =========
# need this since will assert helium triplet lines that depend on stable soln
iterate
constant temper 7500
database h-like element hydrogen levels resolved 10
no level2
no induced processes (OK)
#
# commands controlling output =========
save performance "hhe_outpp.per"
save overview "hhe_outpp.ovr" last
save dr "hhe_outpp.dr" last
#
# hhe_outpp.in
# class limit
# ======================================
#
```

This tests the total emission from a spherical pure hydrogen Stromgren sphere using the outward only approximation. The conservation of the total number of ionizing photons, and the emitted spectrum, are all checked.

---

hhe_outppff.in

plane parallel filling factor pure H, He gas

```
title plane parallel filling factor pure H, He gas
#
# commands controlling continuum =========
ionization -2
blackbody 40000
#
# commands for density & abundances =========
hden 5
init file "hheonly.ini"
#
# commands controlling geometry =========
filling factor -1
sphere
#
# other commands for details =========
# need this since will assert helium triplet lines that depend on stable soln
iterate
constant temper 7500
no level2
no induced processes (OK)
database h-like element hydrogen levels resolved 10
#
# commands controlling output =========
save performance "hhe_outppff.per"
save overview "hhe_outppff.ovr" last
save dr "hhe_outppff.dr" last
#
# helium lines
# hhe_outppff.in
# class limit
# ======================================
#
```

This is a plane-parallel constant temperature cloud with only hydrogen and helium. The gas has a filling factor of 0.1. Induced processes are turned off and a large H atom is used so that the hydrogen recombination spectrum will be close to

Case B. The calculation stops beyond the hydrogen ionization front, because of the stop efrac command (it needs this since this is a constant temperature calculation, so the usual lower-temperature stopping criterion does not apply). The asserts confirm that energy is conserved and that the hydrogen spectrum is correct.

---

hhe_outsp.in

spherical conservation and H-like emission for H, He

```
title spherical conservation and H-like emission for H, He
#
# commands controlling continuum =========
ionization -2
blackbody 40000
#
# commands for density & abundances =========
hden 5
init file "hheonly.ini"
#
# commands controlling geometry =========
radius 13
sphere static
#
# other commands for details =========
iterate
diffuse outward only
constant temper 7500
no level2
no induced processes (OK)
database h-like element hydrogen levels resolved 10
#
# commands controlling output =========
save performance "hhe_outsp.per"
save overview "hhe_outsp.ovr" last
save dr "hhe_outsp.dr" last
#
# helium lines
#
# hhe_outsp.in
# class limit
# ======================================
#
```

This tests a spherical cloud with only hydrogen and helium. Diffuse fields are transferred with the outward only approximation. The asserts check that the ionizing radiation is conserved.

---

hii_blister.in

Lexington 1995 dust-free hii blister region

```
title Lexington 1995 dust-free hii blister region
#
# commands controlling continuum =========
# a simple blackbody
blackbody 40000
# the flux of H-ionizing photons
phi(h) 13.0
# add the CMB after hot star shape & luminosity specified
CMB
#
# commands for density & abundances =========
```

```
hden 4
init file="ism.ini"
# HII region abundance but no dust
abundances hii region no grains
abundances he=1 c=1 n=1 o=1 ne=1 mg=.0001 si=.01 s=1 cl=1 ar=1
continue fe=.001
#
# commands controlling geometry =========
sphere
#
# other commands for details =========
# this is to desaturate Lya to prevent excited state photoionization
# from being important - the other codes did not include this important
# physical process
turbulence 10 km/s
# must iterate since optically thick
iterate
#
# commands controlling output =========
normalize to "Ca B" 4861.32A
# the normalizing line is not defined on the emergent line stack
print lines emergent off
print line faint .01
print line sum
Blnd 5875.66A
blnd 2326
blnd 1335
blnd 1909
N 2 6583.45
N 2 6548.05
n 3 57.3238m
blnd 7325
blnd 3727
O 3 51.8004m
o 3 5006.84
o 3 4958.91
Ne 2 12.8101m
Ne 3 15.5509m
Ne 3 3868.76A
Ne 3 3967.47A
S 3 18.7078m
S 3 9530.62
S 3 9068.62
s 4 10.5076m
end of lines
set blend "HepsNe3" 3968
Ne 3 3967.47
H 1 3970.07
end of lines
save performance "hii_blister.per"
save overview last "hii_blister.ovr"
save dr last "hii_blister.dr"
save results last "hii_blister.rlt"
print line optical depths
#
#
# hii_blister.in
# class hii
# ======================================
```

This is one of the test cases from the Lexington Meeting suite of nebulae (Ferland et al. 1995). It is a grain-free hii_blister HII region, similar to inner regions of the Orion Nebula, except for the absence of grains. The set of lines entered with the print line sum command lists the most powerful coolants in this model. This is one of the tabulated quantities in the Lexington Meeting, and is a fundamental test of energy conservation in the code. The ratio of the sum of these lines to Hb is equivalent to the Stoy ratio, used for determining stellar temperatures.

The "dielec kludge 0" command is to turn off my estimates of the DR rates for those elements that had none. This was only to allow comparison with other calculations that did not make similar estimates. For an actual calculation I would not

include this command, since the guesses are better than nothing.

the turbulence is to stop the balmer lines from becoming optically thick since few other codes include an actual H atom, but use case b instead. The Orion HII region does have an observed turbulence of about 8 km/s.

This calculation stops near the H+ - H0 ionization front, where the temperature falls below the default lowest temperature of 4000 K. This model would have continued into the PDR had a lower temperature been specified with the STOP LOWEST TEMP command.

---

hii_coolstar.in

dust free cool HII region model, Lexington 1995

```
title dust free cool HII region model, Lexington 1995
#
# commands controlling continuum =========
black body, T = 20000 K
q(h) 49
# add the CMB after hot star shape & luminosity specified
CMB
#
# commands for density & abundances =========
hden = 2
init file="ism.ini"
abund He=-1 C=-3.6576 N=-4.39794 O=-3.481146 ne=-4.30103 mg=-8
continue si=-8 s=-5.04576 cl=-7 ar=-8 fe=-8
#
# commands controlling geometry =========
radius = 18.477121
sphere
# this is to go deep to pick up all H recombs
stop efract -2
stop temperature 1000
#
# other commands for details =========
# must iterate since fine structure lines are optically thick
iterate
# assume there is neutral gas beyond what we compute
double
#
# commands controlling output =========
print line faint .01
# this is the sum of lines in table 2 of the Lexington meeting
print line sum
N 2 6583.45
N 2 6548.05
blnd 3727
Ne 2 12.8101m
Blnd 6720
S 3 18.7078m
S 3 33.4704m
S 3 9530.62
S 3 9068.62
end of lines
save performance "hii_coolstar.per"
save overview last "hii_coolstar.ovr"
save dr last "hii_coolstar.dr"
save results last "hii_coolstar.rlt"
save continuum last units microns "hii_coolstar.con"
save lines, zone cumulative, "hii_coolstar.cum"
H 1 4861.32A
o 3 5006.84
blnd 3727
O 1 6300.30
```

```
end of lines
#
# Hbeta 4.93E36, L(total)4.30xHbeta
# hii_coolstar.in
# class hii
# ======================================
#
```

This is one of the test cases from the Lexington Meeting suite of nebulae. It is a grain-free HII region ionized by a very cool star. Hydrogen is ionized but not helium so this tests the transport of the H Lyman continuum. The set of lines is entered with the print line sum command to test energy conservation.

---

hii_hiU_StaticSphere_noGrains.in

very high ionization parameter static H II region without dust

```
title very high ionization parameter static H II region without dust
stop efrac -1
stop temperature 3
sphere static
covering factor 0.500
q(H) = 51.340
radius 1.000 linear parsecs
hden 2.
database h-like element hydrogen resolved levels 20
print line pump
iterate to convergence
```

test

```
title test
# IMF slope: 2.35 Mup=120 Mlow=0.1 Mo
# Metallicity: z004 ;
# Age = 2.9000 Myrs
print off
interpolate ( 6.5172, -10.0000)
continue (12.2727001 , 18.5331989 ) (12.3306917 , 18.4600873 )
continue (12.3976394 , 18.3696100 ) (12.4768200 , 18.2559724 )
continue (12.5737312 , 18.1106805 ) (12.6986694 , 17.9237063 )
continue (12.8747606 , 17.7132364 ) (13.1757900 , 17.9262936 )
continue (13.4759529 , 18.4762233 ) (13.4776898 , 18.4795692 )
continue (13.4794342 , 18.4830526 ) (13.4811860 , 18.4865412 )
continue (13.4829436 , 18.4900359 ) (13.4847097 , 18.4935365 )
continue (13.4864815 , 18.4970429 ) (13.4882616 , 18.5005546 )
continue (13.4900484 , 18.5040724 ) (13.4918434 , 18.5075965 )
continue (13.4936462 , 18.5111264 ) (13.4954555 , 18.5146620 )
continue (13.4972725 , 18.5182046 ) (13.4990971 , 18.5217529 )
continue (13.5009291 , 18.5253099 ) (13.5027698 , 18.5288689 )
continue (13.5046176 , 18.5324342 ) (13.5064739 , 18.5360110 )
continue (13.5083371 , 18.5395916 ) (13.5102098 , 18.5431760 )
continue (13.5120904 , 18.5467681 ) (13.5139776 , 18.5503718 )
continue (13.5158738 , 18.5539755 ) (13.5177790 , 18.5569388 )
continue (13.5196928 , 18.5608904 ) (13.5216140 , 18.5648526 )
continue (13.5235449 , 18.5688178 ) (13.5254828 , 18.5727940 )
continue (13.5274301 , 18.5767735 ) (13.5293867 , 18.5807617 )
continue (13.5313524 , 18.5847603 ) (13.5333258 , 18.5887622 )
continue (13.5353093 , 18.5927732 ) (13.5373014 , 18.5967928 )
continue (13.5393032 , 18.6008181 ) (13.5413133 , 18.6048488 )
continue (13.5433328 , 18.6088943 ) (13.5453628 , 18.6129424 )
continue (13.5474018 , 18.6169987 ) (13.5494508 , 18.6210632 )
continue (13.5515086 , 18.6251325 ) (13.5535772 , 18.6292082 )
continue (13.5556542 , 18.6332996 ) (13.5577429 , 18.6373981 )
continue (13.5598408 , 18.6415044 ) (13.5619489 , 18.6456182 )
```

```
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continue (13.5948653 , 18.7083589 ) (13.5971520 , 18.7126123 )
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continue (15.3199696 , 20.9990948 ) (15.3230065 , 20.9975905 )
continue (15.3260633 , 21.0006943 ) (15.3291435 , 20.9894352 )
continue (15.3322465 , 20.9904172 ) (15.3353716 , 21.0073845 )
continue (15.3385182 , 21.0069908 ) (15.3416877 , 21.0053318 )
continue (15.3448813 , 21.0134248 ) (15.3480984 , 21.0157185 )
continue (15.3513401 , 21.0042014 ) (15.3546039 , 21.0138094 )
continue (15.3578948 , 21.0175456 ) (15.3612102 , 21.0058195 )
continue (15.3645510 , 21.0063468 ) (15.3679185 , 21.0196084 )
continue (15.3713099 , 21.0178367 ) (15.3747300 , 21.0063706 )
continue (15.3781762 , 21.0126813 ) (15.3816511 , 21.0153272 )
continue (15.3851539 , 21.0105359 ) (15.3886854 , 20.9915584 )
continue (15.3922448 , 20.9563151 ) (15.3958329 , 20.9851882 )
continue (15.3994522 , 20.9978933 ) (15.4031016 , 21.0158556 )
continue (15.4067837 , 20.9968721 ) (15.4104955 , 21.0223135 )
continue (15.4142394 , 21.0222047 ) (15.4180144 , 21.0215109 )
continue (15.4218243 , 21.0271061 ) (15.4256679 , 21.0152727 )
continue (15.4295456 , 21.0248236 ) (15.4334578 , 21.0262241 )
continue (15.4374065 , 21.0303274 ) (15.4413903 , 21.0164613 )
continue (15.4454127 , 21.0290571 ) (15.4494707 , 21.0221481 )
continue (15.4535675 , 21.0338721 ) (15.4577048 , 21.0354687 )
continue (15.4618810 , 21.0099679 ) (15.4660962 , 20.9840066 )
continue (15.4703546 , 21.0193030 ) (15.4746547 , 21.0184895 )
continue (15.4789977 , 21.0059282 ) (15.4833847 , 21.0111914 )
continue (15.4878155 , 20.9634934 ) (15.4922937 , 21.0164097 )
continue (15.4968176 , 21.0031759 ) (15.5013893 , 20.9911616 )
continue (15.5060096 , 20.9684398 ) (15.5106790 , 20.9497798 )
continue (15.5153996 , 20.9306123 ) (15.5201716 , 20.5187147 )
continue (15.5249981 , 20.5149828 ) (15.5298780 , 20.5088732 )
continue (15.5348127 , 20.5026895 ) (15.5398048 , 20.4965167 )
continue (15.5448540 , 20.4890922 ) (15.5499640 , 20.4819935 )
continue (15.5551344 , 20.4695196 ) (15.5603670 , 20.4653689 )
continue (15.5656637 , 20.4524790 ) (15.5710248 , 20.4397668 )
continue (15.5764531 , 20.4273950 ) (15.5819508 , 20.4169112 )
continue (15.5875190 , 20.4100744 ) (15.5931597 , 20.4012568 )
continue (15.5988736 , 20.3955636 ) (15.6046644 , 20.3886029 )
continue (15.6105335 , 20.3827572 ) (15.6158838 , 20.3761773 )
continue (15.6219081 , 20.3694322 ) (15.6286321 , 20.3543073 )
continue (15.6348358 , 20.3504622 ) (15.6411299 , 20.3373556 )
continue (15.6475170 , 20.3322476 ) (15.6539993 , 20.3164550 )
continue (15.6585952 , 20.3008007 ) (15.6639072 , 20.2870590 )
continue (15.6706410 , 20.2683418 ) (15.6774801 , 20.2477458 )
continue (15.6844288 , 20.2425990 ) (15.6914908 , 20.2318864 )
continue (15.6986694 , 20.2238651 ) (15.7059689 , 20.2216289 )
continue (15.7133931 , 20.1938231 ) (15.7209461 , 20.1687242 )
continue (15.7286329 , 20.1404385 ) (15.7364579 , 20.1072712 )
continue (15.7444268 , 20.1031348 ) (15.7525447 , 20.1033898 )
continue (15.7608174 , 20.1028748 ) (15.7675506 , 20.1023320 )
continue (15.7726700 , 20.0828479 ) (15.7778508 , 20.0244241 )
continue (15.7866244 , 19.9959514 ) (15.7955797 , 19.9650485 )
continue (15.8047226 , 19.9331090 ) (15.8140630 , 19.9264220 )
continue (15.8226440 , 19.9209928 ) (15.8323818 , 19.9055285 )
continue (15.8433524 , 19.8730683 ) (15.8515085 , 19.8498471 )
continue (15.8598201 , 19.8266249 ) (15.8693655 , 19.8017786 )
continue (15.8802235 , 19.7733768 ) (15.8913601 , 19.7440281 )
continue (15.9027897 , 19.7066073 ) (15.9133396 , 19.6723264 )
continue (15.9241526 , 19.6358988 ) (15.9352417 , 19.6031699 )
continue (15.9479040 , 19.5812323 ) (15.9609467 , 19.5585046 )
continue (15.9743938 , 19.5305784 ) (15.9882699 , 19.4824727 )
continue (15.9982541 , 19.4486510 ) (16.0055280 , 19.4271399 )
continue (16.0144239 , 19.4018320 ) (16.0235035 , 19.3761200 )
continue (16.0319939 , 19.3522018 ) (16.0398621 , 19.3302289 )
continue (16.0478782 , 19.3079525 ) (16.0552177 , 19.2876509 )
continue (16.0618481 , 19.2693807 ) (16.0672271 , 19.2461043 )
continue (16.0747324 , 19.2139237 ) (16.0850050 , 19.1704315 )
```

```
continue (16.0966111 , 19.1220399 ) (16.1076034 , 19.0769092 )
continue (16.1150944 , 19.0465551 ) (16.1211789 , 17.6391991 )
continue (16.1285156 , 17.5295684 ) (16.1347921 , 17.4372264 )
continue (16.1419637 , 17.3312064 ) (16.1535679 , 17.1636239 )
continue (16.1650662 , 16.9692034 ) (16.1718990 , 16.8543482 )
continue (16.1792788 , 16.7225695 ) (16.1892432 , 16.5336645 )
continue (16.1957862 , 16.4120568 ) (16.2070740 , 16.2067905 )
continue (16.2174655 , 16.0226717 ) (16.2210672 , 15.9599413 )
continue (16.2293388 , 15.7813512 ) (16.2377724 , 15.6005237 )
continue (16.2456064 , 15.4356819 ) (16.2567129 , 15.2070487 )
continue (16.2673055 , 14.9943570 ) (16.2759698 , 14.7987223 )
continue (16.2859284 , 14.5310628 ) (16.2978436 , 14.2190644 )
continue (16.3089121 , 13.9369976 ) (16.3205741 , 13.6476827 )
continue (16.3313139 , 13.3881549 ) (16.3413692 , 13.1509343 )
continue (16.3500405 , 12.9508027 ) (16.3549320 , 12.8396239 )
continue (16.3612102 , 12.6987923 ) (16.3682553 , 12.4682923 )
continue (16.3726745 , 12.3112294 ) (16.3806055 , 12.0335586 )
continue (16.3929606 , 11.6114940 ) (16.4056758 , 11.1899262 )
continue (16.4199161 , 10.7326810 ) (16.4338514 , 10.2998297 )
continue (16.4446053 , 9.9753257 ) (16.4531562 , 9.7229785 )
continue (16.4606228 , 9.5066902 ) (16.4682203 , 9.2903934 )
continue (16.4785607 , 8.9416311 ) (16.4869261 , 8.4270799 )
continue (16.4940975 , 7.9941810 ) (16.5060096 , 7.2913992 )
continue (16.5182572 , 6.5892987 )continue ( 22.38, -10.0000)
print on
#
save performance "hii_hiU_StaticSphere_noGrains.per"
save overview "hii_hiU_StaticSphere_noGrains.ovr"
save dr "hii_hiU_StaticSphere_noGrains.dr"
#
#
#
#
#
#
#
# H II region
```

This model was added to have at least one sim with a very high ionization parameter and a grain-free static closed geometry to maximize line trapping.

---

hii_icf.in

HII region with negative He/H ICF

```
title HII region with negative He/H ICF
#
# commands controlling continuum =========
# this is the result of this command
# table star mihalas 46000
# and makes it possible to run these orion sims without
# installing the stellar atmosphere files
table SED "star_mihalas_46000.dat"
ionization parameter -2.
# add the CMB after hot star shape & luminosity specified
CMB
#
# commands for density & abundances =========
hden 3
init file "ism.ini"
abundances ism no grains
grains no qheat single
metals and grains 0.320
#
# commands controlling geometry =========
```

```
stop efrac -3
stop temperature 15
sphere
#
# other commands for details =========
failures 1
#
# commands controlling output =========
save performance "hii_icf.per"
save overview "hii_icf.ovr" last
save dr "hii_icf.dr" last
#
# hii_icf.in
# class hii
# ======================================
```

This is an example of an H II region irradiated by a hard stellar continuum - one of the Mihalas NLTE stars. The hard continuum produces a negative He/H ionization correction factor, as discussed in Ballantyne, Ferland & Martin (2000). >>refer HeI icf by Ballantyne,D.R., Ferland, G.J., & Martin, P.G., 2000, ApJ 536, 773-777

---

hii_paris.in

"New" Paris meeting HII region

```
title "New" Paris meeting HII region
# "standard" HII region model of the Pequignot Meudon Conference
#
# commands controlling continuum =========
black body, T = 40000 K radius = 12.113943
# add the CMB after hot star shape & luminosity specified
CMB
#
# commands for density & abundances =========
hden = 2
init file="ism.ini"
element aluminium on
element helium abundance -1
element carbon abundance -3.6576
element nitrogen abundance -4.39794
element oxygen abundance -3.481146
element neon abundance -4.30103
element magnesium abundance -8
element aluminium abundance -8
element silicon abundance -8
element sulphur abundance -5.04576
element chlorine abundance -7
element argon abundance -8
element iron abundance -8
#
# commands controlling geometry =========
radius = 18.477121
sphere
# next two to make sure we pick up all possible H recombination
set temperature floor 1000
# make sure sim goes very deep into cold gas
stop temperature 100K
stop efrac -2
#
# other commands for details =========
# must iterate since fine structure lines are optically thick
iterate
database h-like element hydrogen levels resolved 10
#
# commands controlling output =========
normalize to "Ca B" 4861.32A
```

```
# the normalizing line is not defined on the emergent line stack
print lines emergent off
print column densities
print line optical depths
print line faint 0.01
print line sum
Blnd 5875.66A
blnd 2326
blnd 1909
n 2 121.769m
N 2 6583.45
N 2 6548.05
n 3 57.3238m
blnd 3727
o 3 5006.84
o 3 4958.91
O 3 51.8004m
O 3 88.3323m
Ne 2 12.8101m
Ne 3 15.5509m
Ne 3 3868.76A
Ne 3 3967.47A
Blnd 6720
S 3 18.7078m
S 3 33.4704m
S 3 9530.62A
S 3 9068.62
s 4 10.5076m
end of lines
save performance "hii_paris.per"
save overview last "hii_paris.ovr"
save each cooling last "hii_paris.cole"
save cooling last "hii_paris.col"
save hydrogen 21 cm last "hii_paris.21cm"
save results last "hii_paris.rlt"
save dr last "hii_paris.dr"
save linelist "hii_paris.lin" "LineList_HII.dat" last no hash column
# this is to confirm that this commnand works
save lines emissivity "hii_paris.str" last
H 1 4861.32A
end lines
#
table lines "LineList_HII.dat"
# hii_paris.in
# class hii
# ======================================
#
```

This is one of the "standard" models computed at the Paris and Lexington meetings on photoionization and shock calculations. a bable in hazy compares the predictions of the current version of CLOUDY with predictions of a few of the other codes. It is necessary to iterate since some fine structure lines are optically thick. The set of lines entered with the print line sum command is used to obtain the total luminosity in detected lines, a measure of the Stoy temperature.

Checks:
- Hb close to case B, Q(H) 4861, intensities.
- Enter answers in Table Error! Reference source not found..

---

hii_Um3.in

H II region sim from Christophe Morriset's ionization paramter family

```
title H II region sim from Christophe Morriset's ionization paramter family
set save prefix "hii_Um3"
```

```
Blackbody 56000
ionization parameter = -3.000
hden = 3
abundances HII region
cosmic ray background
element limit off -8
print line optical depth
iterate
#
#
save last continuum ".con" units microns
save last overview ".ovr"
save performance ".per"
#
# hii_Um3.in
# class hii
# ==========================
```

This is one of three tests suggested by Christophe Morisset to span the range of ionization parameter on a BPT diagram

---

hii_Um35.in

H II region sim from Christophe Morriset's ionization paramter family

```
title H II region sim from Christophe Morriset's ionization paramter family
set save prefix "hii_Um35"
Blackbody 56000
ionization parameter = -3.5
hden = 3
abundances HII region
cosmic ray background
element limit off -8
print line optical depth
iterate
#
#
save last continuum ".con" units microns
save last overview ".ovr"
save performance ".per"
#
# hii_Um3.in
# class hii
# ==========================
```

This is one of three tests suggested by Christophe Morisset to span the range of ionization parameter on a BPT diagram

---

hii_Um385.in

H II region sim from Christophe Morriset's ionization paramter family

```
title H II region sim from Christophe Morriset's ionization paramter family
set save prefix "hii_Um385"
Blackbody 56000
ionization parameter = -3.85
hden = 3
abundances HII region
cosmic ray background
element limit off -8
print line optical depth
iterate
#
```

```
#
save last continuum ".con" units microns
save last overview ".ovr"
save performance ".per"
#
# hii_Um3.in
# class hii
# ==========================
```

This is one of three tests suggested by Christophe Morisset to span the range of ionization parameter on a BPT diagram

---

hlike_c.in

H-like C VI case B

```
title H-like C VI case B
#
# commands controlling continuum =========
table agn
ionization parameter 3
#
# commands for density & abundances =========
hden = 8
init file="ism.ini"
element carbon abundance 1
set eden 9
#
# commands controlling geometry =========
set dr -18
stop zone 1
#
# other commands for details =========
case b hummer no photoionization
no induced processes (OK)
constant temperature = 1.e5
#
# commands controlling output =========
save overview "hlike_c.ovr"
save performance "hlike_c.per"
save results "hlike_c.rlt"
#
# hlike_c.in
# class limit
# ======================================
#

This test case compares the predictions of the multi-level H-like CVI atom
with the Storey and Hummer (1995) results. The set dr command sets the
zone thickness to 1 cm. The case b command sets Lyman line optical depths
to very large values.
Checks:
- Neutral fractions
- H* emissivity
- Relative line intensities
```

---

hlike_o.in

H-like O VIII case B

```
title H-like O VIII case B
#
```

```
# commands controlling continuum =========
table agn
ionization parameter 4
#
# commands for density & abundances =========
hden = 8
init file="ism.ini"
element oxygen abundance 1
set eden 9
#
# commands controlling geometry =========
# set following so the n^2 dr is unity
set dr -18
stop zone 1
#
# other commands for details =========
case b hummer no photoionization
no induced processes (OK)
constant temperature = 1.e5
# Resolve O 8 Lya doublet
database h-like lyman extra resolution 0.01
database h-like oxygen resolved levels 10
database h-like oxygen collapsed levels 10
#
# commands controlling output =========
print lines sort wavelength
print lines column
save overview "hlike_o.ovr"
save performance "hlike_o.per"
save results "hlike_o.rlt"
#
# hlike_o.in
# class limit
# ======================================
#

This test case compares the predictions of the multi-level H-like O VIII atom
with the Storey and Hummer (1995) results. The set dr command sets the
zone thickness to 1 cm. The case b command sets Lyman line optical depths
to very large values.
Checks:
- Neutral fractions
- H* emissivity
- Relative line intensities
```

---

igm_lalpha.in

Ly alpha forest cloud

```
title Ly alpha forest cloud
#
# commands controlling continuum =========
# ionized by cosmic background
# plus quasar/starburst continuum
cmb z=2
table hm05 z = 2
#
# commands for density & abundances =========
hden -2
#
# commands controlling geometry =========
stop "H" column density 15
#
# other commands for details =========
#
# commands controlling output =========
```

```
print line faint -1
set save prefix "igm_lalpha"
save performance ".per"
save overview last ".ovr"
save dr last ".dr"
save results last ".rlt"
#
# on 05 aug 29 changed from old background command to
# cmb 2 plus hm05 z=2 background - all results changed substantially
# igm_lalpha.in
# class igm
# ======================================
#

This example demonstrates the behavior of the code in the low-density limit.
The ionizing source is the cosmic background at a redshift of z = 2.
The cloud is assumed to be optically thin to ionizing radiation,
in keeping with the Gunn-Peterson test, so the double command is included,
and an iteration is performed to converge the optical depth scale.
Continuum fluorescent excitation of lines is important because the cloud
is optically thin.
```

This sim corrects line intensities for isotropic continua. Its sister sim, igm_lalpha_noisosub.in, computes intensities uncorrected for isotropic continua.

---

igm_lalpha_hm12.in

Ly alpha forest cloud

```
title Ly alpha forest cloud
#
# commands controlling continuum =========
# ionized by cosmic background
# plus quasar/starburst continuum
cmb z=2
table hm12 z = 2
#
# commands for density & abundances =========
hden -2
#
# commands controlling geometry =========
stop neutral column density 15
#
# other commands for details =========
#
# commands controlling output =========
print line faint -1
set save prefix "igm_lalpha_hm12"
save performance ".per"
save overview last ".ovr"
save dr last ".dr"
save results last ".rlt"
#
# igm_lalpha_hm12.in
# class igm
# ======================================
#

This example demonstrates the behavior of the code in the low-density limit.
The ionizing source is the cosmic background at a redshift of z = 2.
The cloud is assumed to be optically thin to ionizing radiation,
in keeping with the Gunn-Peterson test, so the double command is included,
and an iteration is performed to converge the optical depth scale.
Continuum fluorescent excitation of lines is important because the cloud
is optically thin.
```

This sim corrects line intensities for isotropic continua. Its sister sim, igm_lalpha_noisosub_hm12.in, computes intensities uncorrected for isotropic continua.

---

igm_lalpha_noisosub.in

Ly alpha forest cloud

```
title Ly alpha forest cloud
#
# commands controlling continuum =========
# ionized by cosmic background
# plus quasar/starburst continuum
cmb z=2
table hm05 z = 2
#
# commands for density & abundances =========
hden -2
#
# commands controlling geometry =========
stop neutral column density 15
#
# other commands for details =========
#
# commands controlling output =========
print line faint -1
no lines isotropic continuum subtraction
set save prefix "igm_lalpha_noisosub"
save performance ".per"
save overview last ".ovr"
save dr last ".dr"
save results last ".rlt"
#
# on 05 aug 29 changed from old background command to
# cmb 2 plus hm05 z=2 background - all results changed substantially
# igm_lalpha_noisosub.in
# class igm
# ======================================
#

This example demonstrates the behavior of the code in the low-density limit.
The ionizing source is the cosmic background at a redshift of z = 2.
The cloud is assumed to be optically thin to ionizing radiation,
in keeping with the Gunn-Peterson test, so the double command is included,
and an iteration is performed to converge the optical depth scale.
Continuum fluorescent excitation of lines is important because the cloud
is optically thin.
```

This sim computes line intensities not corrected for isotropic continua (see the "no lines..." command above). Its sister sim, igm_lalpha.in, computes intensities corrected for isotropic continua.

---

igm_lalpha_noisosub_hm12.in

Ly alpha forest cloud

```
title Ly alpha forest cloud
#
# commands controlling continuum =========
# ionized by cosmic background
# plus quasar/starburst continuum
cmb z=2
table hm12 z = 2
```

```
#
# commands for density & abundances =========
hden -2
#
# commands controlling geometry =========
stop neutral column density 15
#
# other commands for details =========
#
# commands controlling output =========
print line faint -1
no lines isotropic continuum subtraction
set save prefix "igm_lalpha_noisosub_hm12"
save performance ".per"
save overview last ".ovr"
save dr last ".dr"
save results last ".rlt"
#
# igm_lalpha_noisosub_hm12.in
# class igm
# ======================================
#

This example demonstrates the behavior of the code in the low-density limit.
The ionizing source is the cosmic background at a redshift of z = 2.
The cloud is assumed to be optically thin to ionizing radiation,
in keeping with the Gunn-Peterson test, so the double command is included,
and an iteration is performed to converge the optical depth scale.
Continuum fluorescent excitation of lines is important because the cloud
is optically thin.
```

This sim computes line intensities not corrected for isotropic continua (see the "no lines..." command above). Its sister sim, igm_lalpha_hm12.in, computes intensities corrected for isotropic continua.

---

igm_perseus.in

Perseus cluster

```
title Perseus cluster
# model of IGM in Perseus galaxy cluster inspired by Hitommi spectroscopy
# RAD affects the intensity of 2e Fe Fe24 X
# w 1.8504 A
# X 1.8554 A
# y 1.8595 A
# z 1.8682 A
# doublet ratio affected by line optical depths 2025A&A...694L..13G
# Fe 26 1.77802A
# Fe 26 1.78337A
set save prefix "igm_perseus"
# improve continuum resolution and use all levels for Fe23+
init "XRISM.ini"
#
# assume gas is in collisional equilibrium
coronal 4.6e7K
#
# commands for density & abundances =========
hden -1.5
#
stop column density 24.5
# no scattering escape intensity
#
# RAD occurs with default setup
# following would turn off RAD effect, included if commented out
# set UTA off
# RAD occurs with first ionization since large Li-like abundace,
```

```
# second has little RAD since 3e density is small
element iron ionization 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.01 0 0 0
# element iron ionization 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1.5 0 0 0
# adjust models to get higher accuracy
database H-like element iron resolved levels 10
database H-like element iron collapsed levels 50
database He-like element iron resolved levels 10
database He-like element iron collapsed levels 50
iterate to convergence
#
# commands controlling output =========
print line column
print line sort wavelength
print line faint -2
print line faint off
#print line sort intensity
normalize "Fe25" 1.85040A 1
save overview ".ovr"
save performance ".per"
save element oxygen ionization ".oxy"
save element iron ionization ".fe"
save performance ".per"
#
#
#
#
#
#
#
#
#
#
#
#
#
#
#
#
****************************
# agn_erseus.in, hot gas in the Perseus galaxy cluster
# class igm
# ==================================
#
```

This is inspired by Hitomi observations of the Fe complex in Perseus and has been developed by Priyanka Chakraborty as part of her thesis. The 1e and 2e resonance lines are optically thick so the 1e Ka doublet ratio is not 2:1 and RAD affects one member of the 2d Ka multiplet

---

igm_primal.in

cloud with primordial abundances exposed to background at Z=10

```
title cloud with primordial abundances exposed to background at Z=10
#
# commands controlling continuum =========
background, redshift= 10
# background due to agn from Haardt & Madau 1996 ApJ, 461, 20
# this sets both continuum shape and intensity, actually for z=2
table HM96 old
#
# other commands for details =========
# put in a velocity field to stop Lya from causing stability problems
turbulence 20 km/s
# do a second iteration to establish that it is optically thick downstream
iterate
```

```
# this sim should run cleanly - do not accept problems
failures 2
#
# commands for density & abundances =========
# this log of the hydrogen density
hden 5
# stored set of primordial abundances
abundances primordial
#
# commands controlling geometry =========
# we want to shielded face to not be exposed to empty space, but rather
# be just very deep in a dense cloud - this prevents lines from freely
# radiating from the shielded face
double optical depths
# set a lower temperature stopping criterion - default is 4000K
stop temperature 30
#
# commands controlling output =========
# don't want to print lots of faint hydrogen lines
print line faint -3
# some output files with info we want to save
save performance "igm_primal.per"
save temperature history "igm_primal_tem.his"
save ionizing continuum "igm_primal.ion"
save hydrogen conditions "igm_primal.mol"
save heating "igm_primal.het"
save dr "igm_primal.dr"
save cooling "igm_primal.col"
save overview "igm_primal.ovr"
save results last "igm_primal.rlt"
#
# igm_primal.in
# class hii pdr igm
# ======================================

This is a high redshift cloud irradiated by the cosmic background and AGN light.
H- absorption of the z=10 cosmic background is a MAJOR heating agent
This model is very sensitive to treatment of Lya destruction, since resulting
J-bar is major destruction process for H-, which is the H2 formation route.
Lya ots oscillations could develop and are damped by not reevaluating H-
photo rate after first n times, as in hmole.c
```

---

igm_z3.in

redshift 1000 recombination epoch

```
title redshift 1000 recombination epoch
#
# commands controlling continuum =========
# a true blackbody radiation field, in strict thermodynamic equilibrium
blackbody 3000 STE
#
# commands for density & abundances =========
hden 0
abundances primordial
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
case b
iterate
#
# commands controlling output =========
normalize lines to "Ca B" 4861.32A
print ages
```

```
print departure coef element hydrogen
print line faint -5
# the normalizing line is not defined on the emergent line stack
print lines emergent off
save overview "igm_z3.ovr"
save performance "igm_z3.per"
save dr "igm_z3.dr"
#
# igm_z3.in
# class limit igm
# ======================================
#
```

This is a model of the universe near the recombination epoch, at a redshift of a thousand. The gas is exposed to a true blackbody at 3000 K, and the abundances are primordial.

---

igm_z3_thick.in

redshift 1000 recombination epoch

```
title redshift 1000 recombination epoch
#
# commands controlling continuum =========
# A true blackbody radiation field, in strict thermodynamic equilibrium.
# This is a resolved variant of igm_z3, which should have uniform conditions.
blackbody 3000 STE
#
# commands for density & abundances =========
hden 0
abundances primordial
#
# commands controlling geometry =========
# stop zone 1
stop thickness 16
stop temperature 0
#
# other commands for details =========
case b
iterate
#
# commands controlling output =========
normalize lines to "Ca B" 4861.32A
print ages
print departure coef element hydrogen
print line faint -5
# the normalizing line is not defined on the emergent line stack
print lines emergent off
save overview "igm_z3_thick.ovr"
save performance "igm_z3_thick.per"
save dr "igm_z3_thick.dr"
#
# igm_z3_thick.in
# class limit igm
# ======================================
#
```

This is a model of the universe near the recombination epoch, at a redshift of a thousand. The gas is exposed to a true blackbody at 3000 K, and the abundances are primordial.

This is a spatially-resolved variant of igm_z3, which should have uniform conditions throughout the depth.

---

ism.in

cloud irradiated by ism background

```
title cloud irradiated by ism background
#
# commands controlling continuum =========
# this uses the Black continuum with no H-ionizing radiation,
# and with background cosmic rays
cmb
table ism
extinguish by a column of 22
# need cosmic rays to provide ionization to the chemistry
cosmic rays, background
#
# commands for density & abundances =========
hden 0
init file="ism.ini"
abundances ism
#
# commands controlling geometry =========
# set sphere since matter in all directions
sphere
stop temperature linear 10
stop thickness 0.1 linear parsecs
#
# other commands for details =========
# this prevents continuum pumping from exciting H0
Database H-like Lyman pumping off
# this is to converge optical depths
iterate
# this should have no effect since T is larger than 100 K
set temperature floor 100K
#
# commands controlling output =========
# this model has no heavy element molecules, because H2 does not
# really fully form, since Lyman bands are not self-shielded
normalize to "C 2" 157.636m
print line pump
save performance "ism.per"
save overview "ism.ovr" last
save dr "ism.dr"
save heating "ism.het"
save coolign "ism.col"
save continuum "ism.con" units microns last
save continuum "ism.con-no-iso" units microns last no isotropic
#
# ism.in
# class ism
# ======================================
```

TODO - look at temperature struture - it has jitter at about the level of convergence, up and down. Temp jitter caused by eden jitter. This model is nearly isothermal, jitter measures noise in solver, and is great chance to pin this down.

This is a test of the behavior of the code in the extreme of photoionization by a relatively hard continuum, at low densities. The continuum is the galactic background, attenuated by a column density of 10^22 cm-2. Ionization by galactic background cosmic rays is included. Database H-like Lyman pumping off appears since this region is deep in the ISM, and the Lyman lines are quite thick. This example checks whether the ionization balance, thermal balance, and electron density sum, are performed correctly in this limit.

Checks:
- Numerical stability of solution
- Thickness exact

---

ism_cosmicray.in

background cosmic ray ionization by suprathermal electrons only

```
title background cosmic ray ionization by suprathermal electrons only
#
# commands controlling continuum =========
# background CR H0 ionization rate should be 2.5e-17 s^-1,
# Williams et al. ApJ, 503, 689
cosmic rays, background
# this will be VERY faint black 50000
ionization parameter -25
black 50000
#
# commands for density & abundances =========
hden 5
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
iterate
set temperature floor 1000 K
# turn off molecules to test only ions
no molecules
# must turn off charge transfer and its heating, which would dominate,
# since we want to test cr heating and ionization
no charge transfer
no ctheat
# must turn of photoionization by recombining species,
# since we want to test cr heating and ionization
no photoionization
# any time photoionization is turned off, it is best to also
# turn off induced processes, which include pumping in the lyman lines
no induced processes
#
# commands controlling output =========
print ages
save overview "ism_cosmicray.ovr"
save performance "ism_cosmicray.per"
#
# ism_cosmicray.in
# class limit
# ======================================
#
```

This test conditions of cosmic ray ionization. Molecules and charge transfer are disabled so that analytical estimates can be made.

`ism_grid.in`

interstellar cloud irradiated by ism background

```
title interstellar cloud irradiated by ism background
#
# commands controlling continuum =========
# this uses the Black continuum with no H-ionizing radiation,
# and with background cosmic rays
table ism
extinguish by a column of 22
cosmic rays background linear 0.1266
#
# commands for density & abundances =========
```

```
hden 0 vary
grid from -3 to 2 in 0.5 dex steps sequential
init file="ism.ini"
# this turns on ism abundances and grains
abundances ism
#
# commands controlling geometry =========
# set sphere since matter in all directions
sphere
stop temperature linear 10
stop thickness 0.1 linear parsecs
stop zone 1
#
# other commands for details =========
# this prevents continuum pumping from exciting H0
Database H-like Lyman pumping off
#
# commands controlling output =========
# this model has no heavy element molecules, because H2 does not
# really fully form, since Lyman bands are not self-shielded
normalize to "C 2" 157.636m
save performance "ism_grid.per"
save pressure "ism_grid.pre" last no hash
save grid "ism_grid.grd" last no hash
save averages "ism_grid.avr" last no hash
temperature hydrogen 1
end of averages
save overview "ism_grid.ovr" last
save dr "ism_grid.dr"
save heating "ism_grid.het" last no hash
save coolign "ism_grid.col" last no hash
save xspec mtable "ism_grid.fit" range 0.1 3 keV
save temperature "ism_grid.tem" last no hash
#
# sert tempe hydro 1 9942 .05 grid 8575 6468 3606 776 304 169 103 66.2 44.1 31.3
#
# ism_grid.in
# class ism
# ======================================
```

this shows an S-curve calculation - make plot showing density as X-axis and gas pressure (nT) as y-axis

the gas is ionized by the galactic background. the density varies between 1e-3 and 100 cm-3. this is the full range found in the diffuse ism. The components that are produced are CNM - cold neutral medium, density ~ 40 cm-3 WNM - n ~ 0.5 cm-3, WIM - warm ionized medium, n ~ 0.25 cm-3 HIM - hot ionized medium, n ~ 1e-3 cm-3, calculation DOES NOT reproduce observed temperature of HIM - we get ~1e4K but observed is ~1e6 K. HIM is shock, not photo, ionized

---

ism_hot_brems.in

generate continuum due to hot ism in high Z,z starburst

```
title generate continuum due to hot ism in high Z,z starburst
set save prefix "ism_hot_brems"
#
# commands controlling continuum =========
# this sets up coronal equilibrium for temperature and continuum
# cloud is predominantly collisionally ionized
coronal equilibrium, t = 1.e6 K
#
# commands for density & abundances =========
# log of hydrogen density (cm-3), by default a constant density model
hden 1
# chemical composition for a well-evolved star cluster with high Z
# the starburst command generates scale factors that will be used to
# multiply the old solar composition, used in ver 84. this is maintain
```

```
# record of physical changes
abundances old solar 84
abundances starburst Z=10 Zsun
#
# commands controlling geometry =========
# the log of the total hydrogen column density, cm-2
stop column density 21
#
# other commands for details =========
# continuum is plotted in Hzay, we me must iterate to predict this
iterate
#
# commands controlling output =========
# normalize to O 7 Lya
normalize to "O 7" 21.6020
# this shortens the printout somewhat
print line faint 1
# output options
save performance ".per"
save continuum last ".con" no title, units keV
save sulphur ionization ".sul"
save overview last ".ovr"
save dr last ".dr"
#save species data sources ".dsource"
# this is only to document the problem described above
#
# ism_hot_brems.in
# class ism
# ======================================
#
```

This model generates a large column constant density cloud similar to the hot phase of the interstellar medium. The continuum is punched to generate one of the figures in Part 2 of Hazy.

There is a strange feature between 1.7e-3A and 2.2e-3A that is the N emission (head starting at 1.7e-3A with O absorption at 2.2e-3A. This model is strongly enriched in heavies so many metal edges, esp O, are optically thick.

>>TODO 1 the guess of the thickness of the first zone is badly too small, because this model is collisionally ionized, and it used Stromgren length - better to use collisional balance and dr - as result of this the model takes far too many zones

---

ism_jura.in

check rate H2 forms on grain surfaces

```
title check rate H2 forms on grain surfaces
#
# commands controlling continuum =========
# first continuum is FIR hot grain continuum produced in
# unmodeled HII Region
blackbody, t = 75 K
intensity 2.7 (total)
# this is hot star continuum
black 30000
intensity 1.90 range 0.4412 to 1 Ryd
# this will remove all ionizing radiation
extinguish 24 0
cosmic rays, background
#
# commands for density & abundances =========
hden 0
grains ism, abundance log 0.16 no qheat
init file="ism.ini"
abundances he= -1.01 c= -3.52 n=-8 o=-3.30 ne=-8 mg=-5.89
continue si= -6.10 s= -5.10 cl=-7 ar=-8 fe= -6.60
```

```
#
# commands controlling geometry =========
sphere
# stop when gas is fully neutral
stop efrac -10
# stop when gas is cold
stop temperature 10 linear
stop zone 1
#
# other commands for details =========
# set the gas temperature
constant temperature 100 K
Database H-like Lyman pumping off
#
# commands controlling output =========
normalize to "c 2" 157.636m
# uv lines are strongly pumped by stellar continuum, break out contribution
print line pump
print line optical depths
print ages
save overview "ism_jura.ovr"
save performance "ism_jura.per"
save hydrogen 21 cm last "ism_jura.21cm"
#
# ism_jura.in
# class limit
# ======================================
#
```

This model started out life as the Tielens & Hollenbach 1985 pdr. The density was set to unity and the incident radiation field adjusted so that the two default grains have temperatures near 100K. The model asserts that the H2 formation rate on grain surfaces is close to the # >>refer H2 grain physics Jura, M., 1975, ApJ, 197, 575 rate.

---

ism_opacity.in

generate standard ISM opacity curve

```
title generate standard ISM opacity curve
#
# commands controlling continuum =========
table agn
ionization parameter -3
#
# commands for density & abundances =========
grains no qheat
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
iterate
#
# commands controlling output =========
save overview "ism_opacity.ovr"
save performance "ism_opacity.per"
save total opacity last "ism_opacity.opc" units kev
#
# ism_opacity.in
# class limit
# ======================================
#
```

This example creates the file ism_opacity.opc which tabulates the total opacity of the gas as a function of energy. These plots are used in ISM studies to understand the transmission characteristics along a line of sight. The opacity depends on the dust

to gas ratio, the gas phase abundances, and the level of ionization, all of which can be changed by altering parameters given above.

The model is of a 1 cm think parcel of gas which is optically thin in the Lyman continuum and Lyman lines. As a result the hydrogen emission line spectrum is close to case C. The model iterates so that the predicted ionization and emission know about this.

---

ism_set_cr_rate.in

background cosmic ray ionization by suprathermal electrons only

```
title background cosmic ray ionization by suprathermal electrons only
#
# commands controlling continuum =========
cosmic ray rate -16
# this will be VERY faint black 50000
ionization parameter -25
black 50000
#
# commands for density & abundances =========
hden 5
element hydrogen ionization 1 0.00000001
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
constant temperature 1000 K
# turn off molecules to test only ions
# >>chng23 mar 04, add "heavy" option
no molecules heavy
# must turn off charge transfer and its heating, which would dominate,
# since we want to test cr heating and ionization
no charge transfer
no ctheat
# must turn of photoionization by recombining species,
# since we want to test cr heating and ionization
no photoionization
# any time photoionization is turned off, it is best to also
# turn off induced processes, which include pumping in the lyman lines
no induced processes
#
# commands controlling output =========
print ages
save overview "ism_set_cr_rate.ovr"
save performance "ism_set_cr_rate.per"
#
# ism_set_cr_rate.in
# class limit
# ======================================
#
```

This test conditions of cosmic ray ionization. Molecules and charge transfer are disabled so that analytical estimates can be made.

---

limit_casea_h_den13.in

case A

```
title case A
#
# Seaton, M.J, 1959 MN 119, 90,
# 4pi j(beta) 5.56E-26
# for this model total H-beta=4.745
# b(2)=3.73E-3 (3)=3.69E-2 (4)=0.091 (5)=0.145 (6)=0.193
# n.b. very different results if not l-mixed
#
# commands controlling continuum =========
black body, T = 50000 K
ionization parameter -2
#
# commands for density & abundances =========
init file="honly.ini"
#
# commands controlling geometry =========
stop lyman optical depth -6
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature = 10000 K
iterate
#
# commands controlling output =========
# this should make the predicted totl Hbeta near unity for case a
normalize to "H 1" 4861.32A = 1.417
print populations h-like
print departure coefficients
save overview "limit_casea_h_den13.ovr"
save performance "limit_casea_h_den13.per"
#
# limit_casea_h_den13.in
# class limit
# ======================================
#
```

Case A is a mathematical fiction; when the Lyman lines are optically thin continuum pumping must be important if the gas is ionized. Fluorescence is turned off with the no induced processes command. The density is set to a very high value (1015 cm-3) so that the 2s-2p states are well l-mixed, in keeping with standard case A assumptions. As a result, collisional excitation would dominate the level populations, and hydrogen collisions must be turned off with the hydrogen collisions off command. The Ly* optical depth is set to a small value. The set dr command sets the zone thickness to 1 cm. The abundances are set to a very small value so that the electron density is equal to the hydrogen density.
Checks:
- Departure coefficients for H, He levels
- Neutral fractions
- H* emissivity

---

limit_casea_h_den_temp.in

Test model H in Case A limit

```
title Test model H in Case A limit
# grid over nebular range of density and temperature to check Case A H
#
# commands controlling continuum =========
# create H+
laser 2 Ryd
ionization parameter -2
#
# commands for density & abundances =========
init "honly.ini"
hden 2. vary
```

```
grid 2 6 2 sequential
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
no scattering escape
case A hummer no Pdest no photoionization
no induced processes
constant temperature 4. vary
grid 5000K to 20000K step 5000K linear
#
# commands controlling output =========
database H-like print levels
database H-like resolved levels 20
database H-like collapsed levels 30
save grid "limit_casea_h_den_temp.grd"
save overview "limit_casea_h_den_temp.ovr"
save performance "limit_casea_h_den_temp.per"
#
# fixit the wavelength range is adjusted to avoid the Lyman lines
# the Lyman a / 2 photon ratio is wrong at high Temperature -
# is there a temperature dependent branching ratio to n=2 out
# of the collapsed level?
#
# limit_casea_h_den_temp.in
# class limit
# ======================================
#
```

this tests the predicted H I and He I spectra in the Case B limit. The grid is over both density and temperature.

---

limit_caseb_h_den10_temp45.in

the best we can do to predict the H I emission spectrum

```
title the best we can do to predict the H I emission spectrum
#
set save prefix "limit_caseb_h_den10_temp45"
# commands controlling continuum =========
laser 1.4
ionization -1
#
# commands for density & abundances =========
hden 10
set eden 10
init file "honly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
database h-like resolved levels 30
database h-like collapsed levels 70
constant temperature 3e4
case b hummer no photoionzation no pdest
no scattering escape
no induced processes
iterate
#
# commands controlling output =========
print departure h-like hydrogen
print line faint 0.01
print line column
```

```
save overview ".ovr"
save performance ".per"
save diffuse continuum ".dif" last no title units microns
save continuum ".con" last no title units microns
#
```

---

limit_caseb_h_den2_temp37.in

the best we can do to predict the H I emission spectrum

```
title the best we can do to predict the H I emission spectrum
#
# commands controlling continuum =========
laser 1.4
ionization -1
#
# commands for density & abundances =========
hden 100 linear
set eden 2
init file "honly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
database h-like resolved levels 30
database h-like collapsed levels 70
database h-like keep fine structure
constant temper 3.7
case b hummer no photoionzation no pdest
no scattering escape
no induced processes
iterate
#
# commands controlling output =========
print departure h-like hydrogen
print line faint -4
print line column
save overview "limit_caseb_h_den2_temp37.ovr"
save performance "limit_caseb_h_den2_temp37.per"
save diffuse continuum "limit_caseb_h_den2_temp37.dif" last no title units microns
save continuum "limit_caseb_h_den2_temp37.con" last no title units microns
#
#
# limit_caseb_h_den2_temp37.in
# class limit
# ======================================
#
```

This is close to the best and most complete model of H I that the code can do. The predicted results still deviate from the tabulated "Ca B" results because of the principal quantum number specifications (30/70 here; 100/1 in table).

---

limit_caseb_h_den2_temp4.in

the best we can do to predict the H I emission spectrum

```
title the best we can do to predict the H I emission spectrum
#
# commands controlling continuum =========
laser 1.4
```

```
ionization -1
#
# commands for density & abundances =========
hden 100 linear
set eden 2
init file "honly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
database h-like resolved levels 30
database h-like collapsed levels 70
constant temper 4
case b hummer no photoionzation no pdest
no scattering escape
no induced processes
iterate
#
# commands controlling output =========
print departure h-like hydrogen
print line faint 0.01
print line column
save overview "limit_caseb_h_den2_temp4.ovr"
save performance "limit_caseb_h_den2_temp4.per"
save diffuse continuum "limit_caseb_h_den2_temp4.dif" last no title units microns
save continuum "limit_caseb_h_den2_temp4.con" last no title units microns
#
#
# limit_caseb_h_den2_temp4.in
# class limit
# ========================================
#
```

This is close to the best and most complete model of H I that the code can do. The predicted results still deviate from the tabulated "Ca B" results because of the principal quantum number specifications (30/70 here; 100/1 in table).

---

limit_caseb_h_den2_temp45.in

the best we can do to predict the H I emission spectrum

```
title the best we can do to predict the H I emission spectrum
#
set save prefix "limit_caseb_h_den2_temp45"
# commands controlling continuum =========
laser 1.4
ionization -1
#
# commands for density & abundances =========
hden 100 linear
set eden 2
init file "honly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
database h-like resolved levels 30
database h-like collapsed levels 70
constant temperature 3e4
case b hummer no photoionzation no pdest
no scattering escape
no induced processes
```

```
iterate
#
# commands controlling output =========
print departure h-like hydrogen
print line faint 0.01
print line column
save overview ".ovr"
save performance ".per"
save diffuse continuum ".dif" last no title units microns
save continuum ".con" last no title units microns
#
```

---

limit_caseb_h_den2_temp5.in

the best we can do to predict the H I emission spectrum

```
title the best we can do to predict the H I emission spectrum
#
# commands controlling continuum =========
laser 1.4
ionization -1
#
# commands for density & abundances =========
hden 100 linear
set eden 2
init file "honly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
database h-like resolved levels 30
database h-like collapsed levels 70
constant temper 5
case b hummer no photoionzation no pdest
no scattering escape
no induced processes
iterate
#
# commands controlling output =========
print departure h-like hydrogen
print line faint 0.01
print line column
save overview "limit_caseb_h_den2_temp5.ovr"
save performance "limit_caseb_h_den2_temp5.per"
save diffuse continuum "limit_caseb_h_den2_temp5.dif" last no title units microns
save continuum "limit_caseb_h_den2_temp5.con" last no title units microns
#
#
# limit_caseb_h_den2_temp5.in
# class limit
# ======================================
#
```

This is close to the best and most complete model of H I that the code can do. The predicted results still deviate from the tabulated "Ca B" results because of the principal quantum number specifications (30/70 here; 100/1 in table).

---

limit_caseb_h_den2_temp5_coronal.in

the best we can do to predict the H I emission spectrum

```
title the best we can do to predict the H I emission spectrum
#
# commands controlling continuum =========
coronal 5
#
# commands for density & abundances =========
hden 100 linear
set eden 2
init file "honly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
database h-like resolved levels 30
database h-like collapsed levels 70
# Hummer option not included here because the population of the excited states will be zero
case b no photoionzation no pdest
no scattering escape
no induced processes
iterate
#
# commands controlling output =========
print departure h-like hydrogen
print line faint 0.01
print line column
save overview "limit_caseb_h_den2_temp5_coronal.ovr"
save performance "limit_caseb_h_den2_temp5_coronal.per"
save diffuse continuum "limit_caseb_h_den2_temp5_coronal.dif" last no title units microns
save continuum "limit_caseb_h_den2_temp5_coronal.con" last no title units microns
```

---

limit_caseb_h_den4_temp4.in

```
set save prefix "limit_caseb_h_den4_temp4"
#
# Gary tripped over a bug when this command is issued before
# the 'init "honly.ini"' below.
# Keep this command up here to always exercise the fix.
#
save species bands ".band" "FeII_bands.ini" "Fe+"
constant temperature 1e4
hden 4
set eden 4
init "honly.ini"
laser 5
ionization -2
stop zone 1
case B hummer no pdest no photoionization
print departure hydrogen H-like
print departure helium H-like
print line faint -6
print lines column
print lines sort wavelength
atom H-like hydrogen levels resolved 30
atom H-like hydrogen levels collapsed 170
save performance ".per"
```

---

limit_caseb_h_den4_temp45.in

the best we can do to predict the H I emission spectrum

```
title the best we can do to predict the H I emission spectrum
#
set save prefix "limit_caseb_h_den4_temp45"
# commands controlling continuum =========
laser 1.4
ionization -1
#
# commands for density & abundances =========
hden 10000 linear
set eden 4
init file "honly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
database h-like resolved levels 30
database h-like collapsed levels 70
constant temperature 3e4
case b hummer no photoionzation no pdest
no scattering escape
no induced processes
iterate
#
# commands controlling output =========
print departure h-like hydrogen
print line faint 0.01
print line column
save overview ".ovr"
save performance ".per"
save diffuse continuum ".dif" last no title units microns
save continuum ".con" last no title units microns
#
```

---

limit_caseb_h_den4_temp4_Fuji.in

```
set save prefix "limit_caseb_h_den4_temp4_Fuji"
constant temperature 1e4
hden 4
database collisions h-like hydrogen Fujimoto
set eden 4
init "honly.ini"
laser 5
ionization -2
stop zone 1
case B hummer no pdest no photoionization
print departure hydrogen H-like
print departure helium H-like
print line faint -6
print lines column
print lines sort wavelength
atom H-like hydrogen levels resolved 30
atom H-like hydrogen levels collapsed 170
save performance ".per"
```

---

limit_caseb_h_den4_temp4_VR62.in

```
set save prefix "limit_caseb_h_den4_temp4_VR62"
constant temperature 1e4
hden 4
database collisions h-like hydrogen van regemorter
set eden 4
```

```
init "honly.ini"
laser 5
ionization -2
stop zone 1
case B hummer no pdest no photoionization
print departure hydrogen H-like
print departure helium H-like
print line faint -6
print lines column
print lines sort wavelength
atom H-like hydrogen levels resolved 30
atom H-like hydrogen levels collapsed 170
save performance ".per"
```

---

limit_caseb_h_den4_temp4_VS80.in

```
set save prefix "limit_caseb_h_den4_temp4_VS80"
constant temperature 1e4
hden 4
database collisions h-like hydrogen vriens
set eden 4
init "honly.ini"
laser 5
ionization -2
stop zone 1
case B hummer no pdest no photoionization
print departure hydrogen H-like
print departure helium H-like
print line faint -6
print lines column
print lines sort wavelength
atom H-like hydrogen levels resolved 30
atom H-like hydrogen levels collapsed 170
save performance ".per"
```

---

limit_caseb_h_hs87.in

"Case B from Hummer and Storey"

```
title "Case B from Hummer and Storey"
init "honly.ini"
laser 1.1
ionization parameter -1
constant temperature 4
case b hummer no photoionization no pdest
database h-like element hydrogen levels resolved 40
database h-like element hydrogen collapsed levels 70
no induced processes
no level2
no scattering escape
set dr -20
hden 4
stop zone 1
iterate
print populations h-like
print departure h-like
save overview "limit_caseb_h_hs87.ovr"
save performance "limit_caseb_h_hs87.per"
#
#
# limit_caseb_h_hs87.in
# class limit
```

---

limit_caseb_h_lot.in

log density case B, T=500 log n=2

```
title log density case B, T=500 log n=2
#
# commands controlling continuum =========
black body, T = 2.e5 K
ionization parameter -1
#
# commands for density & abundances =========
hden = 2
init file="honly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature = 500
# want H and he fully stripped so we can check H He spectra
case b hummer no photoionization no pdest
no induced processes (OK)
iterate
#
# commands controlling output =========
#
# does not agree with Hummer & Storey, as explained by Ferguson & Ferland
# until 03 jun 02, used small atom, which had smaller differences
# turn on large atom to get best answer
database h-like levels resolved 20
#
save overview "limit_caseb_h_lot.ovr"
save performance "limit_caseb_h_lot.per"
save results "limit_caseb_h_lot.rlt" last
#
```

limit_caseb_h_lot.in # class limit # ===

This tests the ionization and emission line spectrum for H case B at a low density and temperature.

---

limit_caseb_h_n8.in

h_caseb_n8 high density case B

```
title h_caseb_n8 high density case B
#
# commands controlling continuum =========
black body, T = 2.e5 K
ionization parameter -1
#
# commands for density & abundances =========
hden = 8
init file="honly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
# this will not affect the main model, but will test CR heating rate
cosmic ray background
```

```
case b hummer no photoionization no Pdest
no scattering escape
no induced processes (OK)
constant temperature = 20000
iterate
database h-like resolve levels 20
#
# commands controlling output =========
save overview "limit_caseb_h_n8.ovr"
save performance "limit_caseb_h_n8.per"
save results "limit_caseb_h_n8.rlt"
save ionizing continuum "limit_caseb_h_n8.cion"
#
#
# limit_caseb_h_n8.in
# class limit
# ======================================
#
```

This test case compares the predictions of the multi-level hydrogen atom with the Storey and Hummer (1995) results. The set dr command sets the zone thickness to 1 cm. The case b command sets Lyman line optical depths to very large values. Checks:
- Neutral fractions
- H* emissivity
- Relative line intensities

high density causes disagreemeent with HS - collisions

---

limit_caseb_he2_den8.in

limit_caseb_he2_den8 He II case B

```
title limit_caseb_he2_den8 He II case B
#
# commands controlling continuum =========
table agn
ionization parameter 0
#
# commands for density & abundances =========
hden = 8
element helium abundance 1
init file="ism.ini"
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
database h-like element helium levels resolved 30
case b hummer no photoionization no Pdest
no induced processes (OK)
constant temperature = 5e4 K
#
# commands controlling output =========
save overview "limit_caseb_he2_den8.ovr"
save performance "limit_caseb_he2_den8.per"
save results "limit_caseb_he2_den8.rlt"
#
#
# limit_caseb_he2_den8.in
# class limit
# ======================================
#
```

This test case compares the predictions of the multi-level hydrogen atom with the Storey and Hummer (1995) results. The set dr command sets the zone thickness to 1 cm. The case b command sets Lyman line optical depths to very large values.
Checks:
- Neutral fractions
- H* emissivity
- Relative line intensities

---

limit_caseb_he_den.in

Test model H and He atoms in Case B limit

```
title Test model H and He atoms in Case B limit
# grid over nebular range of density and temperature to check Case B H & He
#
# commands controlling continuum =========
laser 5 Ryd
ionization parameter -2
#
# commands for density & abundances =========
init "hheonly.ini"
hden 2. vary
grid 2 6 2 sequential
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
normalize to "He 2" 4685.68A
case b hummer no Pdest no photoionization
no scattering escape
# prevent H I excited levels from being predicted
database H-like element hydrogen resolved levels 3
constant temperature 4.
#
# commands controlling output =========
database H-like print levels
database H-like resolved levels 15
save grid "limit_caseb_he_den.grd"
save overview "limit_caseb_he_den.ovr"
save performance "limit_caseb_he_den.per"
#
#
# limit_caseb_he_den.in
# class limit
# ======================================
#
```

this tests the predicted He II spectra in the Case B limit.

this effectively turns off hydrogen to avoid the problem with every other heII line lying beneath an HI line. this is done by reducing the number of levels for H I.

this asserts the values are within 9% for the standard T = 1e4K and a range of densities. Actually they are all nearly within a few percent except at the lowest temperature of 5000K.

---

limit_caseb_he_den2_temp4.in

the best we can do to predict the HeI emission spectrum

```
title the best we can do to predict the HeI emission spectrum
#
# commands controlling continuum =========
laser 2
ionization -1
#
# commands for density & abundances =========
hden 90 linear
set eden 2
element helium abundance -1
init file "hheonly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr -2.95424
#
# other commands for details =========
database he-like resolved levels 30
database he-like collapsed levels 70
database he-like gbar vriens
constant temper 4
case b hummer no photoionzation no pdest
no scattering escape
no induced processes
iterate
#
# commands controlling output =========
normalize to "Blnd" 4471.50A
print departure he-like helium
print line faint 0.01
# save fits last "limit_caseb_he_den2_temp4.fit"
save overview "limit_caseb_he_den2_temp4.ovr"
save performance "limit_caseb_he_den2_temp4.per"
save diffuse continuum "limit_caseb_he_den2_temp4.dif" last no title units microns
save continuum "limit_caseb_he_den2_temp4.con" last no title units microns
save line list ratio column "limit_caseb_he_den2_temp4.rat" "linelist_he1.dat" last no hash
#
save line populations "limit_caseb_he_den2_temp4.lpop" "linelist_he1.dat" last no hash
# default row option: ratio
save line populations "limit_caseb_he_den2_temp4.row.lpop" "linelist_he1.dat" row last no hash
save line populations "limit_caseb_he_den2_temp4.row_lower.lpop" "linelist_he1.dat" row lower last no
hash
save line populations "limit_caseb_he_den2_temp4.row_upper.lpop" "linelist_he1.dat" row upper last no
hash
save line populations "limit_caseb_he_den2_temp4.row_ratio.lpop" "linelist_he1.dat" row ratio last no
hash
save line populations "limit_caseb_he_den2_temp4.row_tspin.lpop" "linelist_he1.dat" row tspin last no
hash
#
#
# limit_caseb_he_den2_temp4.in
# class limit
# ======================================
#
```

This is close to the best and most complete model of He I that the code can do. The predicted results still deviate from the tabulated "Ca B" results because of the principal quantum number specifications (30/70 here; 100/1 in table).

---

limit_caseb_he_den4_temp4.in

the best we can do to predict the HeI emission spectrum

```
title the best we can do to predict the HeI emission spectrum
#
```

```
# commands controlling continuum =========
laser 2
ionization -1
#
# commands for density & abundances =========
hden 9000 linear
set eden 4
element helium abundance -1
init file "hheonly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr -6.95424
#
# other commands for details =========
database he-like resolved levels 30
database he-like collapsed levels 70
database he-like gbar vriens
constant temper 4
case b hummer no photoionization no pdest
no scattering escape
no induced processes
iterate
#
# commands controlling output =========
normalize to "Blnd" 4471.50A
print departure he-like helium
print line faint 0.01
# save fits last "limit_caseb_he_den4_temp4.fit"
save overview "limit_caseb_he_den4_temp4.ovr"
save performance "limit_caseb_he_den4_temp4.per"
save diffuse continuum "limit_caseb_he_den4_temp4.dif" last no title units microns
save continuum "limit_caseb_he_den4_temp4.con" last no title units microns
save line list ratio column "limit_caseb_he_den4_temp4.rat" "linelist_he1.dat" last no hash
#
#
# limit_caseb_he_den4_temp4.in
# class limit
# ======================================
#
```

This is close to the best and most complete model of He I that the code can do. The predicted results still deviate from the tabulated "Ca B" results because of the principal quantum number specifications (30/70 here; 100/1 in table).

---

limit_caseb_he_den4_temp4_Fuji.in

the best we can do to predict the HeI emission spectrum

```
title the best we can do to predict the HeI emission spectrum
#
# commands controlling continuum =========
laser 2
ionization -1
#
# commands for density & abundances =========
hden 9000 linear
set eden 4
element helium abundance -1
init file "hheonly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr -6.95424
#
# other commands for details =========
```

```
database he-like resolved levels 30
database he-like collapsed levels 70
database collisions he-like helium Fujimoto
constant temper 4
case b hummer no photoionzation no pdest
no scattering escape
no induced processes
iterate
#
# commands controlling output =========
normalize to "Blnd" 4471.50A
print departure he-like helium
print line faint 0.01
save overview "limit_caseb_he_den4_temp4_Fuji.ovr"
save performance "limit_caseb_he_den4_temp4_Fuji.per"
save diffuse continuum "limit_caseb_he_den4_temp4_Fuji.dif" last no title units microns
save continuum "limit_caseb_he_den4_temp4_Fuji.con" last no title units microns
save line list ratio column "limit_caseb_he_den4_temp4_Fuji.rat" "linelist_he1.dat" last no hash
#
#
# limit_caseb_he_den4_temp4.in
# class limit
# ======================================
#
```

This is close to the best and most complete model of He I that the code can do. The predicted results still deviate from the tabulated "Ca B" results because of the principal quantum number specifications (30/70 here; 100/1 in table).

---

limit_caseb_he_den4_temp4_VR62.in

the best we can do to predict the HeI emission spectrum

```
title the best we can do to predict the HeI emission spectrum
#
# commands controlling continuum =========
laser 2
ionization -1
#
# commands for density & abundances =========
hden 9000 linear
set eden 4
element helium abundance -1
init file "hheonly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr -6.95424
#
# other commands for details =========
database he-like resolved levels 30
database he-like collapsed levels 70
database collisions he-like helium van regemorter
constant temper 4
case b hummer no photoionzation no pdest
no scattering escape
no induced processes
iterate
#
# commands controlling output =========
normalize to "Blnd" 4471.50A
print departure he-like helium
print line faint 0.01
save overview "limit_caseb_he_den4_temp4_VR62.ovr"
save performance "limit_caseb_he_den4_temp4_VR62.per"
save diffuse continuum "limit_caseb_he_den4_temp4_VR62.dif" last no title units microns
```

```
save continuum "limit_caseb_he_den4_temp4_VR62.con" last no title units microns
save line list ratio column "limit_caseb_he_den4_temp4_VR62.rat" "linelist_he1.dat" last no hash
#
#
# limit_caseb_he_den4_temp4.in
# class limit
# ======================================
#
```

This is close to the best and most complete model of He I that the code can do. The predicted results still deviate from the tabulated "Ca B" results because of the principal quantum number specifications (30/70 here; 100/1 in table).

---

limit_caseb_he_den4_temp4_VS80.in

the best we can do to predict the HeI emission spectrum

```
title the best we can do to predict the HeI emission spectrum
#
# commands controlling continuum =========
laser 2
ionization -1
#
# commands for density & abundances =========
hden 9000 linear
set eden 4
element helium abundance -1
init file "hheonly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr -6.95424
#
# other commands for details =========
database he-like resolved levels 30
database he-like collapsed levels 70
database collisions he-like helium Vriens
constant temper 4
case b hummer no photoionzation no pdest
no scattering escape
no induced processes
iterate
#
# commands controlling output =========
normalize to "Blnd" 4471.50A
print departure he-like helium
print line faint 0.01
# save fits last "limit_caseb_he_den4_temp4.fit"
save overview "limit_caseb_he_den4_temp4_VS80.ovr"
save performance "limit_caseb_he_den4_temp4_VS80.per"
save diffuse continuum "limit_caseb_he_den4_temp4_VS80.dif" last no title units microns
save continuum "limit_caseb_he_den4_temp4_VS80.con" last no title units microns
save line list ratio column "limit_caseb_he_den4_temp4_VS80.rat" "linelist_he1.dat" last no hash
#
#
# limit_caseb_he_den4_temp4.in
# class limit
# ======================================
#
```

This is close to the best and most complete model of He I that the code can do. The predicted results still deviate from the tabulated "Ca B" results because of the principal quantum number specifications (30/70 here; 100/1 in table).

---

limit_caseb_he_den_temp.in

Test model He atoms in Case B limit

```
title Test model He atoms in Case B limit
# grid over nebular range of density and temperature to check Case B H & He
#
# commands controlling continuum =========
laser 5 Ryd
ionization parameter -2
#
# commands for density & abundances =========
init "hheonly.ini"
hden 2. vary
grid 6 2 -2 sequential
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
normalize to "He 2" 4685.68A
case b hummer no Pdest no photoionization
no scattering escape
# prevent H I excited levels from being predicted
database H-like element hydrogen resolved levels 3
constant temperature 4. vary
grid 5000K to 20000K step 5000K linear
#
# commands controlling output =========
database H-like print levels
database H-like resolved levels 20
save grid "limit_caseb_he_den_temp.grd"
save overview "limit_caseb_he_den_temp.ovr"
save performance "limit_caseb_he_den_temp.per"
#
#
# limit_caseb_he_den_temp.in
# class limit
# ========================================
#
```

this tests the predicted He II spectra in the Case B limit.

this effectively turns off hydrogen to avoid the problem with every other heII line lying beneath an HI line. this is done by reducing the number of levels for H I.

this asserts the values are within 15% for a range of density and temperature. Actually they are all nearly within a few percent except at the lowest temperature. The error greater than 10% occurs at the lowest temperature of 5000K.

`limit_caseb_hhe_den.in`

Test model H and He atoms in Case B limit

```
title Test model H and He atoms in Case B limit
# grid over nebular range of density and temperature to check Case B H & He
#
# commands controlling continuum =========
# create H+ and He+
laser 2.0 Ryd
ionization parameter -2
#
# commands for density & abundances =========
init "hheonly.ini"
```

```
hden 2. vary
grid 2 6 2 sequential
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
print line precision 5
database he-like element helium resolved levels 10
no scattering escape
case b hummer no Pdest no photoionization
constant temperature 4.
#
# commands controlling output =========
database H-like print levels
save grid "limit_caseb_hhe_den.grd"
save overview "limit_caseb_hhe_den.ovr"
save performance "limit_caseb_hhe_den.per"
#
# Case B helium doesn't work well with Hummer option
#
# limit_caseb_hhe_den.in
# class limit
# ======================================
#
```

this tests the predicted H I and He I spectra in the Case B limit.

the grid is over density at the standard temperature of 1e4 K.

---

limit_caseb_hhe_den_temp.in

Test model H and He atoms in Case B limit

```
title Test model H and He atoms in Case B limit
# grid over nebular range of density and temperature to check Case B H & He
#
# commands controlling continuum =========
# create H+ and He+
laser 2 Ryd
ionization parameter -2
#
# commands for density & abundances =========
init "hheonly.ini"
hden 2. vary
grid 2 6 2 ncpus 4
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
print line precision 5
database he-like element helium resolved levels 10
database h-like element hydrogen resolved levels 15
no scattering escape
case b hummer no Pdest no photoionization
constant temperature 4. vary
grid 5000K to 20000K step 5000K linear
#
# commands controlling output =========
database H-like print levels
save grid "limit_caseb_hhe_den_temp.grd"
save overview "limit_caseb_hhe_den_temp.ovr"
save performance "limit_caseb_hhe_den_temp.per"
#
```

```
# Case B helium doesn't work well with Hummer option
#
# limit_caseb_hhe_den_temp.in
# class limit
# ======================================
#
```

this tests the predicted H I and He I spectra in the Case B limit. The grid is over both density and temperature.

---

limit_casec_h_den2.in

H only optically thin in Lyman continuum

```
title H only optically thin in Lyman continuum
#
# commands controlling continuum =========
blackbody 40000
ionization -2
#
# commands controlling geometry =========
stop thickness 16
#
# commands for density & abundances =========
hden 2
init file "honly.ini"
#
# other commands for details =========
iterate
constant temper 10000
no level2
#
# commands controlling output =========
print line inward
save performance "limit_casec_h_den2.per"
save overview "limit_casec_h_den2.ovr" last
save fine optical depths last "limit_casec_h_den2.fin" range 0.9 1.02 every 1
save optical depths last "limit_casec_h_den2.opt"
save continuum "limit_casec_h_den2.con" last units microns
save dr "limit_casec_h_den2.dr" last
#
# limit_casec_h_den2.in
# class limit
# ======================================
#
```

This is a pure hydrogen cloud that is optically thin in the Lyman continuum. The asserts check the emission in several H I lines and continua. This should be close to what really happens in a low column density cloud exposed to a continuum source that does not have strong Lyman lines. (The continuum source used is a pure blackbody, and so has no lines). So this is an example of "Case C" emission >>refer H case C Ferland, G.J. 1999, PASP, 111, 1524

---

limit_casec_h_den5.in

case C

```
title case C
#
# commands controlling continuum =========
black body, T = 50000 K
ionization parameter -2
#
```

```
# commands for density & abundances =========
hden = 5
init file="hheonly.ini"
#
# commands controlling geometry =========
set dr -10
stop zone 1
#
# other commands for details =========
iterate
stop lyman optical depth -6
constant temperature = 10000 K
#
# commands controlling output =========
print h-like populations element hydrogen
print line pump
print departure coefficients element hydrogen
save overview "limit_casec_h_den5.ovr"
save performance "limit_casec_h_den5.per"
#
# limit_casec_h_den5.in
# class limit
# ======================================
#
```

This is Case C, what really happens when optically thin gas is irradiated by a continuum with Lyman line continuum fluorescence allowed.
Checks:
- Departure coefficients for H, He levels
- Neutral fractions
- H* emissivity Case C is described in

>>refer H case C Ferland, G.J. 1999, PASP, 111, 1524

---

limit_compton_hi_t.in

test high-T Compton energy exchange

```
title test high-T Compton energy exchange
#
# commands controlling continuum =========
# as hot as STE bb can be on IEEE 32-bit cpu
# equilibrium temperature should also be 2.51e7
# since gas radiated by true blackbody will equilibriate
# at its temperature
blackbody 7.4 STE
#
# commands for density & abundances =========
hden 10
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
database h-like element oxygen resolved levels 5
database h-like element oxygen collapsed levels 30
set temperature convergence 0.0001
iterate
print h-like departure element oxygen
#
# commands controlling output =========
save overview "limit_compton_hi_t.ovr"
save performance "limit_compton_hi_t.per"
#
```

```
# limit_compton_hi_t.in
# class limit
# ======================================
#
```

This is the highest Compton temperature that can be computed in LTE on an IEEE 32-bit processor. This tests the code in the high-temperature Compton limit. Temperatures as high as 10^10 K can be computed successfully on CPUs with longer word lengths, such as a Cray or the new 64 bit processors.

Checks:
- The equilibrium temperature should be exactly 107.4 K (2.51239107 K).

---

limit_compton_lo_t.in

test low-T Compton energy exchange

```
title test low-T Compton energy exchange
#
# commands controlling continuum =========
black linear 3 lte
brems 5
ionizat -5
#
# commands for density & abundances =========
hden -10
init file "hheonly.ini"
eden -3
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
set temperature convergence 0.0001
iterate 3
#
# commands controlling output =========
save overview "limit_compton_lo_t.ovr"
save performance "limit_compton_lo_t.per"
#
# limit_compton_lo_t.in
# class limit
# ======================================
#
```

This tests the code in the low temperature Compton limit. The gas is illuminated by a 3 K blackbody in thermodynamic equilibrium. The equilibrium temperature should be exactly 3 K. It is necessary to add an extra component of free electrons to test the code in this limit with the eden command. If eden is pushed up too high, ee brems cooling will be artificially boosted compared to other cooling terms and start cooling the gas below 3 K. This is why eden was set to 1e-3 cm^-3 on 20141105.

---

limit_compton_mid_t.in

mid-T Compton energy exchange

```
title mid-T Compton energy exchange
# test of thermal equil in limit_compton_mid_t limit; temp should EXACTLY equal 2E5K
# check continuum partition;
```

```
# energy range, photon densities, luminosities, follow
# 0.25-1. Q=26.6470 L=15.8190 c 1-1.807 Q=26.8867 L=16.3766
# 1.807-4 Q=27.3042 L=17.0948 c 4-20 Q=27.2041 L=17.3179
# 20 -- Q=22.9038 L=22.9038 c total lumin 17.5597
# nufnu(912A) = 1.8029E+16
#
# commands controlling continuum =========
black body t = 2.e5 K lte
#
# commands for density & abundances =========
hden = 6
init file "hheonly.ini"
#
# commands controlling geometry =========
stop zone 1
stop lyman continuum optical depth = -6
set dr 0
#
# other commands for details =========
#
# commands controlling output =========
print line faint .1
print departure coef element hydrogen
save overview "limit_compton_mid_t.ovr"
save performance "limit_compton_mid_t.per"
#
# limit_compton_mid_t.in
# class limit
# ======================================
#
```

This tests the behavior of the code in the Compton limit. The incident continuum is a blackbody in strict thermodynamic equilibrium. Strict thermodynamic equilibrium is expected for all constituents of the gas. The input stream also lists the expected photon fluxes for the incident continuum; this tests the normalization of the continuum, and its distribution. Grains are included to confirm their behavior in the LTE limit. The set dr command sets the zone thickness to 1 cm.

Checks:
- Luminosity, photon flux, over various energy intervals, 4*J at 912143.
- Electron temperature exactly 2*105 K.
- Grain temperature forced to 2*105 K by radiative processes.

---

limit_conserve.in

test that energy is limit_conserved

```
title test that energy is limit_conserved
#
# commands controlling continuum =========
# primary continuum is a hot blackbody
black body, temp=5.5
intensity total -4
# add cosmic background
background
#
# commands controlling geometry =========
# don't stop the calculation until all energy used up
# in order to check energy conservation
stop temperature 3 linear
# cloud will go very deep with temperature near 3K without this
stop thickness 18.1
#
# commands for density & abundances =========
metals -0.5
```

```
hden 1.0
constant pressure
#
# other commands for details =========
iterate
# want a clean calculation
failures 3
# this allows for more molecular gas beyond what we model
double optical depths
#
# commands controlling output =========
save performance "limit_conserve.per"
save pressure "limit_conserve.pre"
save pressure history "limit_conserve.his"
save cooling "limit_conserve.col"
save heating "limit_conserve.het"
save dr "limit_conserve.dr"
save overview "limit_conserve.ovr1"
save overview last "limit_conserve.ovr"
save results "limit_conserve.rlt"
save element carbon "limit_conserve.car"
save element neon "limit_conserve.ne"
save element magnesium "limit_conserve.mag"
save element silicon "limit_conserve.sil"
#
# limit_conserve.in
# class hii pdr
# ======================================
```

This checks that energy is limit_conserved. The code always checks that it did not radiate more energy than was absorbed. This calculation extends well past the photo-dissociation zone into fully molecular gas, so that all of the incident radiation is absorbed. Grains, CMB, & CRs are not present so that only the incident radiation field powers the gas.

Small changes can affect this model to surprising extents because of the presence of a major thermal front at the H0 - H+ transition region.

---

limit_eden.in

Martin Gaskell's funny model

```
title Martin Gaskell's funny model
# used to test that electron density convergence is ok
# hydrogen line spectrum strongly pumped by continuum
# all elements > H have HIGH abundances
# ionization of elements Fe, Mg, Si strongly affected
# by charge transfer
#
# commands controlling continuum =========
black 4000
lumin 27.2
#
# commands for density & abundances =========
hden 5.138
abundances all 1000
#
# commands controlling geometry =========
radius 15
stop zone 1
set dr 0
#
# other commands for details =========
constant temper 5500
#
# commands controlling output =========
print line faint -3
```

```
save overview "limit_eden.ovr"
save performance "limit_eden.per"
#
# limit_eden.in
# class limit
# ======================================
#
```

This is mainly a test of the ability of the code to converge a model with a very strange electron density. The electrons are mainly contributed by heavy elements, and the gas is only slightly ionized.

Ionization of elements Fe, Mg, Si strongly affected by charge transfer with other heavy elements.

Checks:
- Electron density is correct.
- Hydrogen line spectrum strongly pumped by continuum.

---

limit_h_induc.in

constant temper black body limit from Ferland and Rees 1988

```
title constant temper black body limit from Ferland and Rees 1988
# tests whether departure coef are forced to unity by induced processes
#
# commands controlling continuum =========
black body, t = 50000 lte
#
# commands for density & abundances =========
hden 10
init file="hheonly.ini"
#
# commands controlling geometry =========
stop lyman continuum optical depth -6
set dr -10
stop zone 1
#
# other commands for details =========
iterate
constant temper 50000
#
# commands controlling output =========
print populations h-like element hydrogen
print heating
print departure coef element hydrogen
print line faint -1
save overview "limit_h_induc.ovr"
save performance "limit_h_induc.per"
#
# limit_h_induc.in
# class limit
# ======================================
#
```

This example tests whether induced processes force level populations of hydrogen to LTE when they are irradiated by a blackbody in strict thermodynamic equilibrium. The density is low enough value for radiation to dominate the rate equations coupling levels with each other and the continuum. The expectation is for all departure coefficients to equal unity.

Checks:
- Departure coefficients exactly unity.
- Grain temperatures are exactly 5*104 K.

limit_hi_ion.in

very high ionization parameter limit

```
title very high ionization parameter limit
# commands controlling continuum =========
table agn
ionization parameter 15
# commands controlling geometry =========
hden 0
stop zone 1
# other commands for details =========
iterate
#
# commands controlling output =========
save overview "limit_hi_ion.ovr"
save performance "limit_hi_ion.per"
save heating "limit_hi_ion.het"
save cooling "limit_hi_ion.col"
#
#
# func_hi_ion.in
# class function
# ======================================
#
```

This tests a limit of very high ionization

---

limit_laser_1.in

test of H ionization in optically thin limit

```
title test of H ionization in optically thin limit
#
# commands controlling continuum =========
laser 1.5 Ryd
phi(h) 10
#
# commands for density & abundances =========
hden 1
init file="hheonly.ini"
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
constant temperature = 4
iterate to convergence
#
# commands controlling output =========
save overview "limit_laser_1.ovr"
save performance "limit_laser_1.per"
save convergence reason "limit_laser_1.cvr"
#
# limit_laser_1.in
# class limit
# ======================================
#
```

This checks the calculation of the hydrogen photoionization equilibrium. The continuum is a laser peaked at 1.5 Ryd, where the hydrogen photoionization cross section is 2.09*10-18 cm-2.

Checks:
- The hydrogen neutral fraction is nearly 2.00*10-4 (not exact since laser has finite width).
- Hb emissivity close to high density case A. The predicted H 1 4861 intensity should be nearly 2.2 times the expected case B intensity.

H cross section is 2.09E-18 cm^2, rec coef is 4.18E-14 answer is neutral fraction 2.00E-4 also checks that only 3 iterations needed

---

limit_laser_2.in

test of H and HeI ionization in optically thin limit

```
title test of H and HeI ionization in optically thin limit
#
# commands controlling continuum =========
laser 2.0 Ryd
intensity -0.3604
#
# commands for density & abundances =========
hden 1
init file="hheonly.ini"
abundances all -10
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature = 4
iterate to convergence
#
# commands controlling output =========
save overview "limit_laser_2.ovr"
save performance "limit_laser_2.per"
#
# limit_laser_2.in
# class limit
# ======================================
#
```

This checks the calculation of the hydrogen and helium photoionization equilibrium. The continuum is a laser peaked at 2.0 Ryd, and so can only ionize hydrogen and atomic helium.

Checks:
- The hydrogen neutral fraction is nearly Ho/H+=4.51*10-4 (not exact since laser has finite width).
- Hb emissivity close to high density case A. The predicted H 1 4861 intensity should be nearly 2.2 times the expected case B intensity.
- Helium ionization should be Heo/He+ = 6.61*10-4.

H cross section is 0.927E-18 cm^2, rec coef is 4.18E-13 answer is Ho/H+ = 4.51e-4 HeI cross section is 6.54E-18 cm^2, rec coef is 4.32E-13 answer is Heo/He+ = 6.61e-5

---

limit_laser_200.in

ionization in Auger-dominated limit

```
title ionization in Auger-dominated limit
#
# commands controlling continuum =========
laser 200 Ryd
phi(h) 10
#
# commands for density & abundances =========
hden 1
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
iterate to convergence
constant temperature = 5
#
# commands controlling output =========
save overview "limit_laser_200.ovr"
save performance "limit_laser_200.per"
#
# limit_laser_200.in
# class limit
# ======================================
#
```

This checks the calculation of ionization equilibrium. The continuum is a laser peaked at 200 Ryd. It asserts ionization of C, O, and Fe. their ionization is dominated by the Auger effect.

Checks: Auger OK

`limit_laser_200_low.in`

test ionization in Auger-dominated limit

```
title test ionization in Auger-dominated limit
#
# commands controlling continuum =========
laser 200 Ryd
phi(h) 5
#
# commands for density & abundances =========
hden 1
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
iterate to convergence
constant temperature = 4
#
# commands controlling output =========
save overview "limit_laser_200_low.ovr"
save performance "limit_laser_200_low.per"
#
#
#
#
#
```

```
# limit_laser_200_low.in
# class limit
# ======================================
#
```

This checks the calculation of ionization equilibrium. The continuum is a laser peaked at 200 Ryd. It asserts ionization of C, O, and Fe. their ionization is dominated by the Auger effect.

Checks: Auger OK

---

limit_laser_3.in

test H and He ionization in optically thin limit

```
title test H and He ionization in optically thin limit
#
# commands controlling continuum =========
laser 4.3 Ryd
phi(h) 10
#
# commands for density & abundances =========
hden 1
abundances all -10
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
iterate to convergence
constant temperature = 4
#
# commands controlling output =========
save overview "limit_laser_3.ovr"
save performance "limit_laser_3.per"
#
# limit_laser_3.in
# class limit
# ======================================
#
```

This checks the calculation of the hydrogen and helium photoionization equilibrium. The continuum is a laser peaked at 4.3 Ryd, where it can fully ionize both hydrogen and helium.

Checks:
- The hydrogen neutral fraction is nearly 4.18*10-4 (not exact since laser has finite width).
- Helium ion: The ratio He+/He++ should be 1.69*10-3 and the ratio Heo/He+ should be 2.86*10-4.
- Hb emissivity should be close to high-density case A. The predicted H 1 4861 intensity should be nearly 2.2 times the expected case B intensity.

H cross section is 1.0E-18 cm^2, rec coef is 4.18E-13 answer is n(Ho)/n(H+)=4.18e-3 HeI cross section is 1.51E-18 cm^2, rec coef is 4.32e-13 answer is n(Heo)/n(He+)=2.86e-4, so Heo/He = 4.83e-7 HeII cross section is 1.30E-18 cm^2, rec coef is 2.20e-12 answer is n(He+)/n(He2+)=1.69e-3

---

limit_lowd0.in

test low density limit

```
title test low density limit
# this and limit_lowdm6 should get same results
#
# commands controlling continuum =========
table agn
ionization parameter -2
#
# commands for density & abundances =========
hden 0
abundances old solar 84
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
iterate
#
# commands controlling output =========
normalize to "H 1" 4861.32A 0.86
print line sort wavelength range 100 1m
save overview "limit_lowd0.ovr"
save performance "limit_lowd0.per"
save cooling last "limit_lowd0.col"
save continuum last "limit_lowd0.con"
#
# all asserts for both sims are in this file
init file="lowd.dat"
#
# limit_lowd0.in
# class limit
# ========================================
#
```

this test case is paired with lowdm6.in both tests read in the same set of asserts, those contained in the file lowd.dat, and they should get exactly the same answer

this is also the test of the print lines intensity command

---

limit_lowden.in

test optically thin model that extends to very low densities

```
title test optically thin model that extends to very low densities
#
# commands controlling continuum =========
table agn
ionization parameter 0
#
# commands for density & abundances =========
hden -2 to the -2 power
init file="ism.ini"
#
# commands controlling geometry =========
sphere
# this will take density down to 1e-8, below stated limit
radius 10 13
#
# other commands for details =========
#
# commands controlling output =========
save performance "limit_lowden.per"
save overview "limit_lowden.ovr" last
#
```

```
# limit_lowden.in
# class limit
# ======================================
#
```

This model is optically thin, with density falling off as inverse square law, so ionization and temperature should be nearly constant. if outer radius increased by 2 dex problem with level3 will appear, several li seq lines (OVI, NeVIII) will fluctuate when density about 1e-9

We do not assert H lines since the cloud is optically thin and takes at least three iterations to converge optical depth scale, That is not the purpose of this sim

---

limit_lowdm6.in

test low density limit

```
title test low density limit
# this and limit_lowd0 should get same results
#
# commands controlling continuum =========
table agn
ionization parameter -2
#
# commands for density & abundances =========
hden -6
abundances old solar 84
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
iterate
#
# commands controlling output =========
normalize to "H 1" 4861.32A 0.86
print line sort wavelength range 100 1m
save overview "limit_lowdm6.ovr"
save performance "limit_lowdm6.per"
save cooling last "limit_lowdm6.col"
save continuum last "limit_lowdm6.con"
#
# all asserts are in this file
init file="lowd.dat"
#
# limit_lowdm6.in
# class limit
# ======================================
#
```

this test case is paired with lowd0.in both tests read in the same set of asserts, those contained in the file lowd.dat, and they should get exactly the same answer

this also tests the print line sort range command

---

limit_lowion.in

test conditions of very low ionization matrix solver

```
title test conditions of very low ionization matrix solver
```

```
#
# commands controlling continuum =========
blackbody 50000
ionization parameter -30
#
# commands for density & abundances =========
hden 2
init file "hheonly.ini"
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
no molecules
constant temperature 100
#
# commands controlling output =========
save overview "limit_lowion.ovr"
save performance "limit_lowion.per"
#
# limit_lowion.in
# class limit
# ======================================
#
```

This model test very low ionization solution of hydrogen and helium.

---

limit_lte_h_t50_cion.in

collisionally ionized H in LTE limit

```
title collisionally ionized H in LTE limit
#
# commands controlling continuum =========
black body, T = 50000 K
ionization parameter -8
#
# commands for density & abundances =========
hden = 20
set eden 20
init file="hheonly.ini"
#
# commands controlling geometry =========
stop lyman optical depth -6
set dr -10
stop zone 1
#
# other commands for details =========
constant temperature = 50000 K
# want pure collisional model
no induced processes (OK)
database h-like collisional excitation off
database h-like collisions l-mixing off
database he-like collisional excitation off
database he-like collisions l-mixing off
database he-like collapsed levels 20
iterate
#
# commands controlling output =========
print h-like departure coefficients hydrogen
print he-like departure coefficients helium
print populations h-like hydrogen
save overview "limit_lte_h_t50_cion.ovr"
save performance "limit_lte_h_t50_cion.per"
#
```

```
# limit_lte_h_t50_cion.in
# class limit
# ======================================
#
```

This is the limiting case pure hydrogen collisional ionization, There are no excitation or l-mixing collisions, so this tests whether collisional ionization - three body recombination works in detailed balance.

---

limit_lte_h_t50_coll.in

collisionally excited H in LTE limit

```
title collisionally excited H in LTE limit
#
# commands controlling continuum =========
black body, T = 50000 K
ionization parameter -8
#
# commands for density & abundances =========
hden = 20
init file="hheonly.ini"
#
# commands controlling geometry =========
stop lyman optical depth -6
stop zone 1
set dr 0
set eden 20
#
# other commands for details =========
no induced processes (OK)
database h-like collisions l-mixing off
database he-like collapsed levels 20
database he-like collisions l-mixing off
constant temperature = 50000 K
iterate
#
# commands controlling output =========
print h-like departure coefficients hydrogen
print h-like populations hydrogen
print he-like departure coefficients helium
save overview "limit_lte_h_t50_coll.ovr"
save performance "limit_lte_h_t50_coll.per"
#
# limit_lte_h_t50_coll.in
# class limit
# ======================================
#
```

This checks that the model H atom goes to LTE at high densities.

chng 06 aug 24, had not included collisional ionization, and so he-like departure coefficients were very large, around 202. comments said there were problems. turned on collisional ionization, no problems noted

chng 06 jul 22 with RP changes in high-n n-changing collisions the rates are now much smaller - needed to change density to be far higher and several quantities changed. at lower density (1e18 cm-3) the populations are very unphysical and runaway maser now occurs. this is only a homework problem and intended to only test n-changing collisions. with higher density this test is done.

---

limit_lte_he1_coll.in

He atom at high densities

```
title He atom at high densities
#
# commands controlling continuum =========
laser 2
ionization -3
#
# commands for density & abundances =========
hden 18
set eden 18
element helium abundance -1
init file "hheonly.ini"
#
# commands controlling geometry =========
stop zone 1
set dr -10
#
# other commands for details =========
database he-like resolved levels 10
database he-like collapsed levels 20
constant temper 20000 K
iterate
#
# commands controlling output =========
print he-like departure helium
normalize to "Blnd" 4471.50A
print line faint -2
save overview "limit_lte_he1_coll.ovr"
save performance "limit_lte_he1_coll.per"
#
# limit_lte_he1_coll.in
# class limit
# ======================================
#
```

test whether he-like ion populations go to lte in high density limit. The level populations should be in LTE, and the departure coefficients should be unity.

---

limit_lte_he1_nomole_iso_force.in

He atom in LTE at high densities, with no molecules, iso forced to LTE

```
title He atom in LTE at high densities, with no molecules, iso forced to LTE
#
# commands controlling continuum =========
blackbody 50000 STE
#
# commands for density & abundances =========
hden 1
# a high he abundance so that it dominates
element helium abundance 18
init file "hheonly.ini"
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
# atom he-like levels 7
# atom he-like collapsed levels 30
no molecules
database h-like levels LTE
database he-like levels LTE
iterate
#
# commands controlling output =========
```

```
print he-like departure helium
print he-like population helium
print h-like departure helium
print h-like population helium
print h-like departure hydrogen
normalize to "Blnd" 4471.50A
print line faint -2
save overview "limit_lte_he1_nomole_iso_force.ovr"
save performance "limit_lte_he1_nomole_iso_force.per"
save heating "limit_lte_he1_nomole_iso_force.het"
save cooling "limit_lte_he1_nomole_iso_force.col"
save dr "limit_lte_he1_nomole_iso_force.dr"
#
# limit_lte_he1_nomole_iso_force.in
# class limit
# ======================================
#
```

test whether a gas dominated by He goes to LTE in high-density limit. The level populations should be in LTE, the departure coefficients should be unity, and the temperature equal to the BB temp.

---

limit_lte_he1_nomole_ste.in

He atom in LTE at high densities, with no molecules

```
title He atom in LTE at high densities, with no molecules
#
# commands controlling continuum =========
blackbody 50000 STE
#
# commands for density & abundances =========
hden 1
# a high he abundance so that it dominates
element helium abundance 18
init file "hheonly.ini"
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
database he-like resolved levels 7
database he-like collapsed levels 30
no molecules
iterate
#
# commands controlling output =========
print he-like departure helium
print he-like population helium
print h-like departure helium
print h-like population helium
print h-like departure hydrogen
normalize to "Blnd" 4471.50A
print line faint -2
save overview "limit_lte_he1_nomole_ste.ovr"
save performance "limit_lte_he1_nomole_ste.per"
save heating "limit_lte_he1_nomole_ste.het"
save cooling "limit_lte_he1_nomole_ste.col"
save dr "limit_lte_he1_nomole_ste.dr"
save species departure "limit_lte_he1_nomole_ste.dep" last all
#
# limit_lte_he1_nomole_ste.in
# class limit
# ======================================
#
```

test whether a gas dominated by He goes to LTE in high-density limit. The level populations should be in LTE, the departure coefficients should be unity, and the temperature equal to the BB temp.

---

limit_lte_he1_nomole_ste_nocoll.in

He atom in LTE at high densities, with no molecules and no collapsed levels

```
title He atom in LTE at high densities, with no molecules and no collapsed levels
#
# commands controlling continuum =========
blackbody 50000 STE
#
# commands for density & abundances =========
hden 1
# a high he abundance so that it dominates
element helium abundance 18
init file "hheonly.ini"
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
no molecules
iterate
#
# commands controlling output =========
print he-like departure helium
print he-like population helium
print h-like departure helium
print h-like population helium
print h-like departure hydrogen
normalize to "Blnd" 4471.50A
print line faint -2
save overview "limit_lte_he1_nomole_ste_nocoll.ovr"
save performance "limit_lte_he1_nomole_ste_nocoll.per"
save heating "limit_lte_he1_nomole_ste_nocoll.het"
save cooling "limit_lte_he1_nomole_ste_nocoll.col"
save dr "limit_lte_he1_nomole_ste_nocoll.dr"
#
# limit_lte_he1_nomole_ste_nocoll.in
# class limit
# ======================================
#
```

test whether a gas dominated by He goes to LTE in high-density limit. The level populations should be in LTE, the departure coefficients should be unity, and the temperature equal to the BB temp.

Level collapse options have been switched off in this, compared to limit_lte_he1_nomole_ste, so effect of including the collapsed levels on LTE can be verified.

---

limit_lte_he1_nomole_ste_nocoll2.in

He atom in LTE for a large range of Te and density, with no molecules and no collapsed levels and no collisions

```
title He atom in LTE for a large range of Te and density, with no molecules and no collapsed levels
and no collisions
#
# commands controlling continuum =========
```

```
blackbody 4.3 STE vary
grid 3.7 to 6.5 step 0.1 sequential
#
# commands for density & abundances =========
hden 1
# a high he abundance so that it dominates
element helium abundance 18 vary
grid 4 to 18 2.0
init file "hheonly.ini"
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
no molecules
database h-like collisions off
database he-like collisions off
set dr -10
#
# commands controlling output =========
print he-like departure helium
print he-like population helium
print h-like departure helium
print h-like population helium
normalize to "Inci" 4860
print line faint -2
# the normalizing line is not defined on the emergent line stack
print lines emergent off
save grid "limit_lte_he1_nomole_ste_nocoll2.grd"
save overview "limit_lte_he1_nomole_ste_nocoll2.ovr"
save performance "limit_lte_he1_nomole_ste_nocoll2.per"
save heating "limit_lte_he1_nomole_ste_nocoll2.het"
save cooling "limit_lte_he1_nomole_ste_nocoll2.col"
save dr "limit_lte_he1_nomole_ste_nocoll2.dr"
#
# >>chng 14 dec 14, Badnell S DR, increase error
# limit_lte_he1_nomole_ste_nocoll2.in
# class limit
# ========================================
#
```

test whether a gas dominated by He goes to LTE in a range of conditions. The level populations should be in LTE, the departure coefficients should be unity, and the temperature equal to the BB temp.

These are STE calculations with no collapsed levels, no collisions, and no molecules, so these models should stringently test the thermodynamic equilibrium limit of radiative coupling terms.

---

limit_lte_he1_ste.in

He atom in LTE at high densities

```
title He atom in LTE at high densities
#
# commands controlling continuum =========
blackbody 50000 STE
#
# commands for density & abundances =========
hden 18
# a high he abundance so that it dominates
element helium abundance 1
init file "hheonly.ini"
#
# commands controlling geometry =========
stop zone 1
#
```

```
# other commands for details =========
database he-like resolved levels 7
database he-like collapsed levels 30
# atom h2 matrix all
iterate
#
# commands controlling output =========
print he-like departure helium
print he-like population helium
print h-like departure helium
print h-like population helium
print h-like departure hydrogen
normalize to "Blnd" 4471.50A
print line faint -2
save overview "limit_lte_he1_ste.ovr"
save performance "limit_lte_he1_ste.per"
save heating "limit_lte_he1_ste.het"
save cooling "limit_lte_he1_ste.col"
save dr "limit_lte_he1_ste.dr"
save species departure "limit_lte_he1_ste.dep" last all
save dominant rates "limit_lte_he1_ste.h2" "H2"
#
# limit_lte_he1_ste.in
# class limit
# ========================================
#
```

test whether a gas dominated by He goes to LTE in high-density limit. The level populations should be in LTE, the departure coefficients should be unity, and the temperature equal to the BB temp.

---

limit_lte_hhe_coll_t50.in

H, He in LTE at high densities

```
title H, He in LTE at high densities
# test from Ferland and Rees 88, collisions drive H to LTE
# collisions should drive all departure coef to unity
#
# commands controlling continuum =========
black body t = 50000
ionization parameter -5
#
# commands for density & abundances =========
hden = 19
init file="hheonly.ini"
set eden 20
#
# commands controlling geometry =========
set dr -10
stop zone 1
stop lyman optical depth -6
#
# other commands for details =========
constant temperature = 50000
iterate
#
# commands controlling output =========
print departure coefficients h-like hydrogen
print populations h-like hydrogen
print departure coefficients h-like helium
print populations h-like helium
print departure coefficients he-like helium
print populations he-like
save overview "limit_lte_hhe_coll_t50.ovr"
save performance "limit_lte_hhe_coll_t50.per"
```

```
save dr "limit_lte_hhe_coll_t50.dr" last
#
# limit_lte_hhe_coll_t50.in
# class limit
# ======================================
#
```

This model is a test of the behavior of hydrogen and helium in the high density, collision dominated, limit. The temperature is preset, the hydrogen density is set to a very high value, and the ionization parameter is very low. The resulting model is collision dominated, so this case checks that the collision physics occurs in detailed balance. The predicted departure coefficients should all equal unity. The set dr command sets the zone thickness to 1 cm.

Checks:
- Hydrogen departure coefficients exactly unity.
- Helium departure coefficients near unity. (Density not high enough to bring helium departure coefficients exactly to unity.)
- H-, H2, H2+ H3+, and HeH+ departure coefficients exactly unity. `

---

limit_lte_hhe_induc.in

radiation dominated H, He gas goes to STE

```
title radiation dominated H, He gas goes to STE
#
# commands controlling continuum =========
black body, t = 50000 STE
#
# commands for density & abundances =========
hden 4
init file="hheonly.ini"
#
# commands controlling geometry =========
stop lyman continuum optical depth -6
set dr -10
stop zone 1
#
# other commands for details =========
iterate
set temperature convergence 0.002
#
# commands controlling output =========
print populations h-like hydrogen
print heating
print departure coef element hydrogen
print line faint -1
save overview "limit_lte_hhe_induc.ovr"
save performance "limit_lte_hhe_induc.per"
#
# limit_lte_hhe_induc.in
# class limit
# ======================================
#
```

This is a H, He-only gas that is optically thin in the Lyman continuum. It is irradiated by a blackbody in strict thermodynamic equilibrium. The tests confirm that the gas temperature equilibriates close to the black body temperature.

---

limit_lte_hhe_ste.in

H, He in STE

```
title H, He in STE
# from Ferland and Rees 1988
# this tests whether thermal processes go to STE
#
# commands controlling continuum =========
black body, t = 50000 STE
#
# commands for density & abundances =========
hden 10
init file="hheonly.ini"
#
# commands controlling geometry =========
stop lyman optical depth -6
set dr -10
stop zone 1
#
# other commands for details =========
iterate
#
# commands controlling output =========
print heating
print populations h-like hydrogen
print departure coef h-like hydrogen
print departure coef he-like helium
save overview "limit_ste_hhe_ste.ovr"
save performance "limit_ste_hhe_ste.per"
#
# limit_ste_hhe_ste.in
# class limit
# ======================================
#
```

This is the ultimate test of the behavior of the code in the strict thermodynamic equilibrium limit. The temperature is not held constant, so the resulting equilibrium temperature determines whether cooling processes are treated properly in the detailed balance limit. The equilibrium temperature should be exactly 5*104 K, and all departure coefficients should equal unity. A small amount of grains are included to check that the grain thermal balance is handled properly in this limit.

Checks:
- Electron temperature exactly 5*104 K.
- Departure coefficients unity.

---

limit_lte_hminus.in

H- goes to LTE

```
title H- goes to LTE
#
# commands controlling continuum =========
# this is a second way to get STE and tests the energy density option
blackbody 5000 energy density 5000K
#
# commands for density & abundances =========
hden 10
#
# commands controlling geometry =========
stop zone 1
set dr 0
#
# other commands for details =========
iterate
constant temperature 5000
#
```

```
# commands controlling output =========
print populations h-like hydrogen
save overview "limit_lte_hminus.ovr"
save performance "limit_lte_hminus.per"
print departure coef element hydrogen
#
# limit_lte_hminus.in
#
# class limit
# ======================================
#
```

This checks that the negative hydrogen ion goes to thermodynamic equilibrium when irradiated by a blackbody in thermodynamic equlibrium. It was originally presented in >>refer H- test Ferland, G. J., & Persson, S. E. 1989, ApJ, 347, 656

---

limit_lte_metal.in

STE with metals

```
title STE with metals
# this tests whether thermal processes go to STE
#
# commands controlling continuum =========
# a dilution factor of 1 is one way to get STE
black body, t = 20000 dilution 1
#
# commands for density & abundances =========
hden 10
abundances starburst 5
#
# commands controlling geometry =========
stop zone 1
stop lyman optical depth -6
set dr -10
#
# other commands for details =========
iterate
#
# commands controlling output =========
print departure coef element hydrogen
print populations h-like hydrogen
save overview "limit_lte_metal.ovr"
save performance "limit_lte_metal.per"
save heating "limit_lte_metal.het" last
save cooling "limit_lte_metal.col" last
#
# limit_lte_metal.in
# class limit
# ======================================
#
```

This checks that the code goes to strict thermodynamic equilibrium for the case of a metal rich gas exposed to a true black body. The many heavy element lines should dominate cooling, so this is a test that the multilevel atoms go to LTE in the radiation-dominated limit.

Checks:
- Temperature should equilibrate at 20000 K.
- Departure coefficients should equal unity.

---

limit_recoil_ion.in

test compton recoil ionization of hydrogen

```
title test compton recoil ionization of hydrogen
#
# commands controlling continuum =========
laser 2000 ryd
ionization parameter -5
#
# commands for density & abundances =========
hden 0
init "honly.ini"
#
# commands controlling geometry =========
set dr 14
stop zone 10
#
# other commands for details =========
iterate
no secondary ionization
constant temperature 1000
#
# commands controlling output =========
save overview "limit_recoil_ion.ovr"
save performance "limit_recoil_ion.per"
#
#
# limit_recoil_ion.in
# class limit
# ======================================
#
```

H ionization is totally due to recoil ionization in this model. The assert checks the final hydrogen ionization.

`limit_strom.in`

pure-H Stromgren sphere

```
title pure-H Stromgren sphere
# the answer is R(Stromgren) = 4.16E17 cm
#
# commands controlling continuum =========
blackbody 50000 K
q(h) 49
#
# commands for density & abundances =========
hden 4
init file "honly.ini"
abundances all -10
#
# commands controlling geometry =========
sphere static
radius 16
stop efrac -0.5
#
# other commands for details =========
no level2
turbulence 20 km/s
constant temper 7500
iterate
#
# commands controlling output =========
save performance "limit_strom.per"
```

```
save overview last "limit_strom.ovr"
save results last "limit_strom.rlt"
save dr last "limit_strom.dr"
#
# limit_strom.in
# class limit
# ======================================
#
```

This case checks that the code computes the geometry and emissivity correctly for a pure hydrogen spherical shell. The low temperature is chosen to avoid collisional ionization. The model stops at the Ho-H+ ionization front. The turbulence is to prevent the Balmer lines from becoming optically thick.
Checks
- Outer radius should be 4.16391017 cm.
- Predicted Hb, case B Hb, and Q(H) Hb, all agree.

---

limit_supra.in

secondary ionization dominated gas

```
title secondary ionization dominated gas
# like SN envelope
#
# commands controlling continuum =========
# this continuum will be VERY faint
table agn
ionization parameter -25
# secondary ioinzations will dominate
set csupra -5
#
# commands for density & abundances =========
hden 5
abundances old solar 84
#
# commands controlling geometry =========
stop temperature 20
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature 1000 K
iterate convergence
#
# commands controlling output =========
print ages
save overview "limit_supra.ovr"
save performance "limit_supra.per"
save heating "limit_supra.het"
save ionizing continuum "limit_supra.ion" last
save molecules "limit_supra.mol"
#
#
# limit_supra.in
# class limit
# ======================================
#
```

This model computes the ionization within cool gas that is totally ionized by suprathermal secondary electrons.

Charge transfer heating is VERY important in this simulation.

---

limit_thick_brems.in

optically thick brems

```
title optically thick brems
#
# check that optically thick brems emission approaches the RJ limit
#
# commands controlling continuum =========
blackbody 2e5
#
# we need to test this command in at least one sim
Xi 3
#
# commands for density & abundances =========
hden 6
#
# commands controlling geometry =========
stop column density 20
#
# other commands for details =========
constant temperature 1e4
iterate 3
set nFnu diffuse outward
set nFnu add 2e-8 ryd
set nFnu add 5e-8 ryd
set nFnu add 1e-7 ryd
set nFnu add 2e-7 ryd
set nFnu add 5e-7 ryd
set nFnu add 1e-6 ryd
set nFnu add 2e-6 ryd
set nFnu add 5e-6 ryd
set nFnu add 1e-5 ryd
set nFnu add 2e-5 ryd
set nFnu add 5e-5 ryd
#
# commands controlling output =========
print line faint -10
save continuum "limit_thick_brems.con" last units microns
save optical depth "limit_thick_brems.opd" last
save overview "limit_thick_brems.ovr"
save dr "limit_thick_brems.dr"
#
# commands giving the asserts =========
#
#
# limit_thick_brems.in
# class limit
# ======================================
#
```

At some point we had a major bug affecting the optically thick part of the radio free-free emission. This sim checks that the optically thick emission from a plane-parallel slab has the correct Rayleigh-Jeans shape. This implies that at long wavelengths nuFnu should vary as lambda^3.

---

limit_vbhum.in

compare with Van Blerkom and Hummer exact RT results

```
title compare with Van Blerkom and Hummer exact RT results
#
# commands controlling continuum =========
blackbody 50000 K
phi(h) 12.30103
```

```
# commands for density & abundances =========
hden 4
init "honly.ini"
abundances all -10
#
# commands controlling geometry =========
stop efrac -0.5
#
# other commands for details =========
diffuse ots
no level2 lines
constant temper 4
iterate
#
# commands controlling output =========
save performance "limit_vbhum.per"
save overview last "limit_vbhum.ovr"
save dr last "limit_vbhum.dr"
#
#
# limit_vbhum.in
#
# class limit
# ======================================
#
```

This is a test of the treatment of the diffuse fields, their transfer, and their effects on the ionization structure of a nebula. The comparison is made against the exact calculation published by Van Blerkom and Hummer (1967). The geometry is open, that is, similar to that assumed in most BLR calculations.

>>refer H ionization Van Blerkom, D., & Hummer, D. G. 1967, MNRAS, 137, 353

The diffuse ots command is entered in order to reproduce the Van Blerkom and Hummer results. The default assumption, outward only, does not agree as well. I changed the default from OTS to outward only to be in better agreement with predictions by Harrington and Rubin at the Lexington meeting. They have not checked whether their codes are in agreement with the Van Blerkom and Hummer paper.

Checks:
- Neutral fraction at illuminated face 5.8*10-4.
- Location of ionization front at 7.8*1016 cm.
- 34He 1 486134 and 34CA B 486134 agree; both slightly lower than 34Q(H) 486134.
- Answers with OTS agree with 1967 results.

test hydrogen ground state rec effic against vb+h exact results this is their case e) - "zero condition" their answer for H0/Htot at the illuminated edge is approx 5.8E-4, and a Stromgren radius of approximately 7.7E16 cm

---

limit_veryveryfast.in

very fast simulation for Purify/valgrind

```
title very fast simulation for Purify/valgrind
#
# commands controlling continuum =========
table agn
ionization parameter -2
#
no file opacity
set dr 0
#
# commands for density & abundances =========
hden 9
```

```
init file "hheonly.ini"
element oxygen on
#
# commands controlling geometry =========
stop zone 1
#
# other commands for details =========
no level 2
constant temperature 4
database h-like levels small
database he-like levels small
#
# commands controlling output =========
save overview "limit_veryveryfast.ovr"
save performance "limit_veryveryfast.per"
save dr last "limit_veryveryfast.dr"
#
#
# limit_veryveryfast
# class limit
# ======================================
#
```

This is meant to be a very fast calculation to use when running extensive debug-enabled runtimes.

---

lya-21cm-constant.in

test effect of lya pump on spin temperature

```
title test effect of lya pump on spin temperature
#
# commands controlling continuum =========
#
table ism
extinguish column 22
CMB, z=0
#
# commands for density & abundances =========
# set the density and composition, ism with grains
#
hden 2
abundance ism
#
# other commands for details =========
#
# this is an important ionization source
cosmic rays background
# optical depth
double
iterate
turbulence 3 km/s
# stopping criteria
stop temperature 3K linear
stop neutral hydrogen column density 18
#
# command exercised =========
#
set lya 21cm constant
#
# commands controlling output =========
#
set save prefix "lya-21cm-constant"
save hydrogen 21cm ".21cm" last
save hydrogen lya ".lya" last
save overview ".ovr" last
```

```
#
#
#
#
#
# # ======================================
```

This is one of the sims employed by Shaw, Ferland, & Hubeny 2017, ApJ, 843, 149. It exercises the Snu=constant case to column density of 1e18, while the original paper used a 1e20 stopping criterion.

---

lya-21cm-excitation.in

test effect of lya pump on spin temperature

```
title test effect of lya pump on spin temperature
#
# commands controlling continuum =========
#
table ism
extinguish column 22
CMB, z=0
#
# commands for density & abundances =========
# set the density and composition, ism with grains
#
hden 2
abundance ism
#
# other commands for details =========
#
# this is an important ionization source
cosmic rays background
# optical depth
double
iterate
turbulence 3 km/s
# stopping criteria
stop temperature 3K linear
stop neutral hydrogen column density 18
#
# command exercised =========
#
set lya 21cm excitation
#
# commands controlling output =========
#
set save prefix "lya-21cm-excitation"
save hydrogen 21cm ".21cm" last
save hydrogen lya ".lya" last
save overview ".ovr" last
#
#
#
#
#
# # ======================================
```

This is one of the sims employed by Shaw, Ferland, & Hubeny 2017, ApJ, 843, 149. It exercises the Snu~B(Texc) case to column density of 1e18, while the original paper used a 1e20 stopping criterion.

---

lya-21cm-kinetic.in

test effect of lya pump on spin temperature

```
title test effect of lya pump on spin temperature
#
# commands controlling continuum =========
#
table ism
extinguish column 22
CMB, z=0
#
# commands for density & abundances =========
# set the density and composition, ism with grains
#
hden 2
abundance ism
#
# other commands for details =========
#
# this is an important ionization source
cosmic rays background
# optical depth
double
iterate
turbulence 3 km/s
# stopping criteria
stop temperature 3K linear
stop neutral hydrogen column density 18
#
# command exercised =========
#
set lya 21cm kinetic
#
# commands controlling output =========
#
set save prefix "lya-21cm-kinetic"
save hydrogen 21cm ".21cm" last
save hydrogen lya ".lya" last
save overview ".ovr" last
#
#
#
#
#
# # ======================================
```

This is one of the sims employed by Shaw, Ferland, & Hubeny 2017, ApJ, 843, 149. It exercises the Snu~B(Tkin) case to column density of 1e18, while the original paper used a 1e20 stopping criterion.

---

nlr_lex00.in

NLR model for Lexington 2000 Meeting

```
title NLR model for Lexington 2000 Meeting
#
# commands controlling continuum =========
phi(h) 12.47712
# shape of continuum is interpolated table
interpolate (0 -10) (0.08 -10) (0.1 1) (3676 -4.935) (4700 -11)
continue (4750 -20) (7.4e6 -30)
#
# commands controlling geometry =========
stop column 22
#
```

```
# commands for density & abundances =========
hden 4
init file="c84.ini"
abundances He=-1 c=-3.52 n=-4 o=-3.097 ne=-4 na=-9
continue mg=-4.523 al=-8 si=-4.523 s=-4.824 ar=-9 ca=-8 fe=-8 ni=-9
#
# other commands for details =========
iterate
#
# commands controlling output =========
print line faint .01
# add sum of these lines to printout for Stoy ratio
print line sum
H 1 1215.67A
Blnd 5875.66A
blnd 1909
blnd 1549
N 2 6583.45
N 2 6548.05
n 3 57.3238m
blnd 1750
blnd 1486
O 1 6300.30
o 1 63.1679m
blnd 3727
blnd 1666
O 3 51.8004m
o 3 5006.84
o 3 4958.91
blnd 1402
Ne 3 15.5509m
Ne 3 3868.76A
Ne 3 3967.47A
Blnd 2424
Ne 5 3425.88A
Ne 5 3345.82A
blnd 2798
si 2 34.8046m
Blnd 6720
S 3 18.7078m
S 3 9530.62
S 3 9068.62
S 4 10.5076m
end of lines
#
save performance "nlr_lex00.per"
save overview last "nlr_lex00.ovr"
save dr last "nlr_lex00.dr"
save results last "nlr_lex00.rlt"
#
# nlr_lex00.in
# class nlr
# ======================================
```

This is one of the test cases from the Lexington (1993) Meeting suite of nebulae. It is a grain-free NLR model.

---

nlr_liner.in

NLR liner model

```
title NLR liner model
# a constant pressure (gas+radiation) model of a nlr_liner cloud
# in the spirit of Ferland and Netzer 1983
#
# commands controlling continuum =========
```

```
table agn
ionization parameter -3
#
# commands for density & abundances =========
hden 6
init file "ism.ini"
abundances old solar 84
metals 0.3
#
# commands controlling geometry =========
stop thickness 16.3
stop column density 23
constant pressure
#
# other commands for details =========
#
# commands controlling output =========
save performance "nlr_liner.per"
save overview last "nlr_liner.ovr"
save element nitrogen last "nlr_liner.nit"
save dr last "nlr_liner.dr"
save results last "nlr_liner.rlt"
#
# nlr_liner.in
# class nlr
# ======================================
```

This is a model somewhat like the Liner parameters proposed by Ferland and Netzer (1983). A second iteration is performed to allow the calculation of the line radiation pressure.

>>refer nlr_liner model Ferland, G. J., & Netzer, H. 1983, ApJ, 264, 105

---

nlr_liner_grains.in

liner model with grains

```
title liner model with grains
#
# a constant pressure (gas+radiation) model of a liner cloud
# in the spirit of Ferland and Netzer 1983
#
# commands controlling continuum =========
ionization parameter -3
table agn
#
# commands for density & abundances =========
hden 6
# this turns on both grains and depleted abundances
abundances ism no grains
grains ism no qheat single
init file "ism.ini"
#
# commands controlling geometry =========
stop column density 23
#
# other commands for details =========
constant pressure
#
# commands controlling output =========
save performance "nlr_liner_grains.per"
save overview last "nlr_liner_grains.ovr"
save dr last "nlr_liner_grains.dr"
save continuum last "nlr_liner_grains.con" units microns
save results last "nlr_liner_grains.rlt"
#
```

```
# nlr_liner_grains.in
# class nlr
# ======================================
#
```

This is a model somewhat like the Liner parameters proposed by Ferland and Netzer (1983). A second iteration is performed to allow the calculation of the line radiation pressure. It includes grains and is so more realistic.

>>refer liner model Ferland, G. J., & Netzer, H. 1983, ApJ, 264, 105

---

nlr_paris.in

Paris meeting NLR model

```
title Paris meeting NLR model
#
# commands controlling continuum =========
interpolate (0 -10) (0.073 -10) (0.074 1) (7352 -4)
continue (7400 -15) (7.353e6 -20)
ionization parameter -2
#
# commands controlling geometry =========
stop lyman continuum optical depth 4
#
# commands for density & abundances =========
hden 3
init file="c84.ini"
abund He=-1 C=-3.5229 N=-4. O=-3.22185 ne=-3.82391 na=-8 mg=-4.5229 al=-8
continue si=-4.5229 s=-4.82391 ar=-8 ca=-8 fe=-7 ni=-8
#
# other commands for details =========
# this large group of lines are turned off so that the model runs
# 30 percent faster - lines are mainly fuv and x-ray, which we will
# not track in this model
no level2
iterate
database h-like element helium levels resolved 10
#
# commands controlling output =========
save performance "nlr_paris.per"
save overview last "nlr_paris.ovr"
save dr last "nlr_paris.dr"
save results last "nlr_paris.rlt"
#
# nlr_paris.in
# class nlr
# ======================================
```

This is the NLR model presented in the Meudon meeting on model nebulae. The init file is entered to make the code behave more like version 84.

Checks:
- init file works

---

nova_dqher.in

cold nova shell

```
title cold nova shell
```

```
# Ferland et al. 1984 DQ Her
# model of room temperature ionized cloud arund old nova DQ Her
# roughly that of
# tests behaviour of code at very low temperatures
#
# commands controlling continuum =========
# flat continuum, followed by nu^-2 power law
interpolate (0 0) (0.3 0) (8.e6 -14.8)
luminosity total 34
#
# commands for density & abundances =========
hden = 2.
abundances nova
grains no qheat single
#
# commands controlling geometry =========
filling factor 0.667
covering factor 0.667
radius 16.5682 , thickness = 16.14613
# need this since gas is so cool
stop temp = 100
#
# other commands for details =========
cosmic rays background
iterate
turbulence 300
database h-like element hydrogen levels resolved 15
database h-like element helium levels resolved 15
#
# commands controlling output =========
normalize to label="CaBo" 4861.32A intensity 1.169
print line all
# the normalizing line is not defined on the emergent line stack
print lines emergent off
save performance "nova_dqher.per"
save overview last "nova_dqher.ovr"
save results last "nova_dqher.rlt"
save dr last "nova_dqher.dr"
save transmitted continuum "nova_dqher.trn" last
#
# nova_dqher.in
# class nova
# ======================================
#
```

This tests the code39s behavior in the limit posed by the metal rich low density nebula surrounding DQ Her (Ferland et al. 1984).
Checks:
- Thickness exact
- Thermal stability High-Z gas ionization at low temperature

---

nova_photos.in

dense nova photosphere

```
title dense nova photosphere
set save prefix "nova_photos"
#
# commands controlling continuum =========
# this is the result of this command
# table star kurucz 35000; use old atlas atmosphere
# and makes it possible to run sims without
# installing the stellar atmosphere files
# set SED of central star
table SED "star_kurucz_35000.dat"
```

```
# set luminosity of central star
absolute bolometric magnitude -8.1
#
# commands for density & abundances =========
#
# commands controlling geometry =========
#
# other commands for details =========
iterate to convergence
#
# commands controlling output =========
print line faint -1
save performance ".per"
save overview ".ovr" last
save convergence reason ".cvg" no hash
save results ".rlt" last
save dr ".dr" last
save heat ".het" last
save cool ".col" last
#
# nova_photos.in
# class nova
# ======================================
#
```

this model is intensely affected by continuum pumping of atoms. The hydrogen ionizaiton is by lyman line pumping, followed by photoionization from excited states.

---

optimize_phymir.in

test phymir optimizers

```
title test phymir optimizers
# spectrum computed with hden 5, temp 4
# subplex, phymir, powell
#
# commands controlling continuum =========
black 40000 K
ionization par -3
#
# commands for density & abundances =========
hden 4 vary
init file "hheonly.ini"
element oxygen on
#
# commands controlling geometry =========
Case B
stop zone 1
#
# other commands for details =========
optimize tolerance 0.03
constant temper 4.3 vary
optimize phymir
optimize iteration 100
# the following spectrum was derived by running this sim at hden 5 and t=4
# resulting eden was 5.039 and T=4, which we shall assert that we find
# >>chng 06 apr 03, backdate to old [OII] As and rederive spectrum
optimize lines
O 2 3728.81 0.1567
O 2 3726.03 0.4087
Blnd 7323 0.4344
Blnd 7332 0.3577
O 3 5006.84 3.8117
O 3 4363.21 0.0368
end of lines
```

```
#
# commands controlling output =========
print line faint -2
#
save overview "optimize_phymir.ovr"
save performance "optimize_phymir.per"
#
# optimize_phymir.in
# class optimizer
# ======================================
#
```

This checks whether the optimizer can recover a known solution. The line spectrum was calculated at T = 1e4 K and and n_H=1e5 cm^-3, and resulted in the given electron density. The model optimize_subplex.in is a copy of this file.

---

optimize_subplex.in

test subplex optimizer

```
title test subplex optimizer
# spectrum computed with hden 5, temp 4
# subplex, phymir, amoeba, powell
#
# commands controlling continuum =========
black 40000 K
ionization par -3
#
# commands for density & abundances =========
hden 4 vary
init file "hheonly.ini"
element oxygen on
#
# commands controlling geometry =========
Case B
stop zone 1
#
# other commands for details =========
constant temper 4.3 vary
optimize subplex
optimize iteration 100
optimize tolerance 0.01
# the following spectrum was derived by running this sim at hden 5 and t=4
# resulting eden was 5.039 and T=4, which we shall assert that we find
# >>chng 06 apr 03, backdate to old [OII] As and rederive spectrum
optimize lines
O 2 3728.81 0.1567
O 2 3726.03 0.4087
Blnd 7323 0.4344
Blnd 7332 0.3577
O 3 5006.84 3.8117
O 3 4363.21 0.0368
end of lines
#
# commands controlling output =========
print line faint -2
#
save overview "optimize_subplex.ovr"
save performance "optimize_subplex.per"
#
# optimize_subplex.in
# class optimizer
# ======================================
#
```

This checks whether the optimizer can recover a known solution. The line spectrum was calculated at T = 1e4 K and and n_H=1e5 cm^-3, and resulted in the given electron density. The model optimize_phymir.in is a copy of this file.

---

orion_hii_open.in

conditions similar to Orion nebula blister

```
title conditions similar to Orion nebula blister
# orion hii region with open geometry
#
# commands controlling continuum =========
# SED of central star
table SED "star_kurucz_39600.dat"
# its flux of H-ionizing photons
phi(h) 13.0
#
# this is to include velocity field in radiative transfer
turbulence 8 km/sec no pressure
#
# commands for density & abundances =========
hden 4
abundances hii region no grains
grains orion
#
# commands controlling geometry =========
cosmic rays, background
constant pressure
# this is the account for continued matter beyond i front
double optical depths
#
# other commands for details =========
iterate 2
#
# commands controlling output =========
print line faint -5
# print lines as surface brightness
print lines surface brightness arcsec
print line optical depths
# want to print line intensities are surface brightness, per arcsec^2
print lines surface brightness arcsec
save pressure "orion_hii_open.pre"
save performance "orion_hii_open.per"
save overview last "orion_hii_open.ovr"
save dr last "orion_hii_open.dr"
save continuum last "orion_hii_open.con" units microns
save transmitted continuum last "orion_hii_open.trn"
save overview last "orion_hii_open.ovr"
save fine opacity last "orion_hii_open.opc" range 0.7 0.9 ryd
save element nitrogen last no hash "orion_hii_open.nit"
save lines, array "orion_hii_open.lina" units microns last no hash
save line emissivity "orion_hii_open.ems" last no hash emergent
H 1 4861.32A
O 3 5006.84A
Blnd 5199A
O 1 6300.30A
O 1 63.1679m
end of lines
save linelist "orion_hii_open.lin" "LineList_HII.dat" last no hash emergent absolute
#
# orion_hii_open.in
# class hii
# ======================================
```

This is a model similar in spirit to the blister geometry HII region model computed by Baldwin et al. (1991). Size-resolved Orion grains are included. The constant pressure command does a hydrostatic equilibrium structure. The predicted emission-

line spectrum is affected by the reddening of the internal grains. The resulting t2 analysis produces artificial results as a result. This has an open geometry, the original BFM paper was a closed geometry. (This makes little difference). Background cosmic rays are also included although these should have little effect on warm ionized gas. The emission line spectrum is given in surface brightness units, as in the BFM paper.

---

orion_hii_pdr.in

constant pressure H+ region/pdr

```
title constant pressure H+ region/pdr
#
# commands controlling continuum =========
# the incident continuum is two parts
# star and flux of photons striking it
# this is the photosphere of the OVI star, its temperature and Q(H)
# this is the result of this command
# table star kurucz 39600 K
# and makes it possible to run these orion sims without
# installing the stellar atmosphere files
table SED "star_kurucz_39600.dat"
Q(H) 49
# this adds the observed hot brems, its temperature and the flux of
# photons striking the cloud
brems 6
phi(h) 10
# add cosmic rays, which are important in the pdr
cosmic rays, background
#
# commands controlling geometry =========
# this sets the separation from the star and the face of the cloud
radius 17.4507
# this turns off the stop temperature opption
# the sim will not stop due to temperature
stop temperature off
# this is typical of a gmc, larson 1981
stop total hydrogen column density 23
# this sets the thickness of the HII region & PDR
stop thickness 0.5 linear parsec
# constant total pressure, so like orion_hii_open
constant pressure
# this will result in a milli gauss B-field in molecular region
magnetic field -5 gauss
# the orion environment full covers the star, so turn on sphere
sphere
# we have a spherical geometry but want to simulate observing
# through a spectrometer's slit. use the aperture
# command for this
aperture beam
#
# other commands for details =========
# mimic existence of unmodeled molecular gas
double
# iterate since lines optically thick
iterate
# the observed microturbulence, partially a flow, so not included in pressure
turbulence 8 km/sec no pressure
# set the line width so lines appear on the save continuum
set save line width 10 km/s
# there should be no failures at all
failures 3
#
# commands for density & abundances =========
# this is the log of the initial H density, cm-3
hden 4
# this will speed up the calculation a bit
```

```
init file="ism.ini"
# this uses HII region abundances, but no grains
abundances hii region no grains
# this turns on orion grains, but leaves quantum heating off to save time
grains orion no qheat
# turn on PAHs, with an abundance that depends on H0 fraction,
# as suggested by long-slit observations of Orion bar,
# with an abundance 3x larger than default built into the code
grains PAH function 3
#
# commands controlling output =========
normalize to "O 1" 63.1679m
# print lots of faint CO lines
print line faint -4
save performance "orion_hii_pdr.per"
save overview last "orion_hii_pdr.ovr"
save heating "orion_hii_pdr.het"
save cooling "orion_hii_pdr.col"
save dr last "orion_hii_pdr.dr"
save results last "orion_hii_pdr.rlt"
save lines, array "orion_hii_pdr.lina" last, units microns
save continuum last "orion_hii_pdr.con" units microns
save hydrogen 21 cm last "orion_hii_pdr.21cm"
save hydrogen lya last "orion_hii_pdr.lya"
save element silicon last "orion_hii_pdr.sil"
save grain extinction last "orion_hii_pdr.grnext"
save grain charge last "orion_hii_pdr.grnchr"
save grain potential last "orion_hii_pdr.grnpot"
save grain temperature last "orion_hii_pdr.grntem"
#
#
#
# orion_hii_pdr.in
# class hii pdr
# ======================================
```

This extends BFM from the H+ region into the PDR as in Abel et al 2005. This is the correct way to do a PDR calcualtion.

>>refer Orion model Baldwin, J., Ferland, G. J., >>refercon Martin, P. G., Corbin, M., Cota, S., Peterson, >>refercon B. M., & Slettebak, A. 1991, ApJ, 374, 580

>>refer physics HII/PDR Abel, N.P., Ferland, G.J., Shaw, G. & >>refercon van Hoof, P.A.M. 2005, ApJS, 161, 65

---

orion_hii_pdr_fast.in

constant gas pressure H+ region/PDR

```
title constant gas pressure H+ region/PDR
# much faster due to physics disabled by fast.ini
#
# commands controlling continuum =========
# the incident continuum is two parts
# star and flux of photons striking it
# this is the result of this command
# table star kurucz 39600 K
# and makes it possible to run these orion sims without
# installing the stellar atmosphere files
table SED "star_kurucz_39600.dat"
Q(H) 49
# add cosmic rays, which are important at depth
cosmic rays, background
# plus hot brems
brems 6
phi(h) 10
#
```

```
# commands for density & abundances =========
hden 4
init file="fast.ini"
abundances hii region no grains
# single sized grain with no quantum heating
grains orion no qheat single
#
# commands controlling geometry =========
radius 17.4507
sphere
# let it go into the molecular cloud
stop temperature 10 linear
# this is roughly the thickness of OMC1
stop thickness 1 linear parsec
# mimic existence of unmodeled molecular gas with double command
double
#
# other commands for details =========
failures 3
iterate
# make constant gas pressure since fast turned off line radiation pressure
constant gas pressure
# the observed microturbulence
turbulence 8 km/sec
# we have a spherical geometry but want to simulate observing
# through a spectrometer's slit. use the aperture
# command for this
aperture beam
#
# commands controlling output =========
normalize to "CaBo" 4861.32A
print line faint -4
# the normalizing line is not defined on the emergent line stack
print lines emergent off
save performance "orion_hii_pdr_fast.per"
save overview last "orion_hii_pdr_fast.ovr"
save heating "orion_hii_pdr_fast.het"
save cooling "orion_hii_pdr_fast.col"
save dr last "orion_hii_pdr_fast.dr"
save results last "orion_hii_pdr_fast.rlt"
save continuum last "orion_hii_pdr_fast.con" units microns
save ionizing continuum last "orion_hii_pdr_fast.ion"
save hydrogen 21 cm last "orion_hii_pdr_fast.21cm"
save hydrogen lya last "orion_hii_pdr_fast.lya"
save element silicon last "orion_hii_pdr_fast.sil"
save element sulphur last "orion_hii_pdr_fast.sul"
#
#
# orion_hii_pdr_fast.in
# class hii pdr
# ======================================
#
```

Orion HII region and PDR, simialr to orion_hii_pdr but much faster because of fast.ini

---

pdr_co_fully.in

H2 and CO in fully molecular limit

```
title H2 and CO in fully molecular limit
# this is a pair with pdr_co_fully_noneq - that tests non equilibrium chem
#
# commands controlling continuum =========
blackbody 5000
luminosity total solar linear 2
```

```
brems 6
luminosity total solar log -2.7
#
# commands for density & abundances =========
# set the density and composition, ism with grains
hden 10
abundances ism no qheat
#
# other commands for details =========
# this is an important ionization source
cosmic ray background
# code will stop at 4000 K by default, lower this temp so we
# can do fully molecular gas
stop temperature 10K linear
#
# commands controlling geometry =========
# the radius and thickness
radius 15.8
stop thickness 6
turbulence 3 km / s
#
# commands controlling output =========
save performance "pdr_co_fully.per"
save overview "pdr_co_fully.ovr"
save molecules "pdr_co_fully.mol"
save dr "pdr_co_fully.dr"
save heating "pdr_co_fully.het"
save cooling "pdr_co_fully.col"
save grain charge "pdr_co_fully.grnchr"
save grain drift "pdr_co_fully.grndft"
save grain temperature "pdr_co_fully.grntem"
save ionization means "pdr_co_fully.ion"
#
#
# gas has more he++ than He+ due to fast charge transfer with co
# neutralizing he+
# pdr_co_fully.in
# class pdr
# ========================================
```

test code in fully molecular limit this is a pair with pdr_co_fully_noneq - that tests non equilibrium chem

---

pdr_co_fully_noneq.in

H2 and CO are fully molecular, non-equilibrium case

```
title H2 and CO are fully molecular, non-equilibrium case
# this is a pair with pdr_co_fully.in, which does not include non-equil chem
#
# commands controlling continuum =========
blackbody 5000
luminosity total solar linear 2
brems 6
luminosity total solar log -2.7
#
# commands for density & abundances =========
# set the density and composition, ism with grains
hden 10
abundances ism no qheat
#
# other commands for details =========
# this is an important ionization source
cosmic ray background
# code will stop at 4000 K by default, lower this temp so we
# can do fully molecular gas
```

```
stop temperature 10K linear
#
# commands controlling geometry =========
# the radius and thickness
radius 15.8
stop thickness 6
turbulence 3 km / s
# this turns on non-equilibrium chemistry as suggested by Federman et al. 1996
set chemistry non equilibrium
#
# commands controlling output =========
save performance "pdr_co_fully_noneq.per"
save overview "pdr_co_fully_noneq.ovr"
save molecules "pdr_co_fully_noneq.mol"
save dr "pdr_co_fully_noneq.dr"
save heating "pdr_co_fully_noneq.het"
save cooling "pdr_co_fully_noneq.col"
save grain charge "pdr_co_fully_noneq.grnchr"
save grain drift "pdr_co_fully_noneq.grndft"
save grain temperature "pdr_co_fully_noneq.grntem"
#
#
# gas has more he++ than He+ due to fast charge transfer with co
# neutralizing he+
# pdr_co_fully_noneq.in
# class pdr
# ========================================
```

test code in fully molecular limit with Federman non-equilibrium chem this is a pair with pdr_co_fully.in, which does not include non-equil chem

---

pdr_coolbb.in

illumination by cool STE blackbody

```
title illumination by cool STE blackbody
# gasis fully molecular, grains should be in STE
#
# commands controlling continuum =========
# illuminate with 120 blackbody in thermodynamic equilibrium
blackbody 120 STE
CMB
#
# commands for density & abundances =========
# density
hden 7
# ism dust and grains
abundances ISM no grains
# dust to gas ratio is 10x standard
grains 1.0
# lowers metals and grains to 1/10 standard, so metals are
# 1/10 solar while dust to gas ratio is galactic
metals and grains 0.1
#
# other commands for details =========
# CO heating sets dr on second iteration, need many zones
set nend 1600
# set background cosmic rays to allow chemistry
cosmic ray background
# we need iterate to convergence here, but that doesn't work for now...
iterate convergence
#
# commands controlling geometry =========
radius 17.5
sphere
```

```
stop temperature 20K linear
stop column density 25.5
# double optical depths in PDR sims, to account for unmodelled
# molecular cloud behind the PDR
double
#
# commands controlling output =========
save performance "pdr_coolbb.per"
save overview "pdr_coolbb.ovr"
save heating "pdr_coolbb.het"
save cooling "pdr_coolbb.col"
save dr "pdr_coolbb.dr"
save grain temperature "pdr_coolbb.grntem"
save convergence reason "pdr_coolbb.cvr"
save lines emissivity "pdr_coolbb.ems"
H2O 212.468m
H2O 160.466m
CO 325.137m
CO 144.745m
CO 118.548m
CN 880.858m
end
#
#
# pdr_coolbb.in
# class pdr
# ======================================
```

This is a dense ISM exposed to a cool blackbody. This tests the ability to converge onto a VERY molecular environment. Nearly all C and H are in CO and H2. Cosmic rays are the main source of heat and ionization.

Continuum pumping of CO followed by collisional deexcitation is a major heating agent across the sim.

---

pdr_dense_persei.in

dense phase zeta persei cloud

```
title dense phase zeta persei cloud
#
# density and abundances ==========
# density of dense phase from Table 2 of Le Petit paper ========
hden 4.3
#
# abundandces from Table 1 of Le Petit paper ==========
element carbon abundance 0.000132 linear
element helium abundance 0.10 linear
element oxygen abundance 0.00032 linear
element nitrogen abundance 0.000075 linear
element sulphur abundance 0.0000186 linear
element silicon abundance 0.000029 linear
# set abundance of all other elements to zero ====================
element copper off
element magnesium off
element manganese off
element sodium off
element chlorine off
element vanadium off
element potassium off
element phosphorous off
element calcium off
element iron off
element zinc off
element neon off
element argon off
element fluorine off
```

```
element aluminum off
element boron off
element lithium off
element beryllium off
element scandium off
element nickel off
element titanium off
element chromium off
element cobalt off
# do not use Federman rates for this model ==============
set federman chemistry off
# use standard ism grain size distribution ============
grains ism
#
# command controlling the continuum, for this model is Draine 1978 field ====
table draine 0.5 linear
# make sure no H-ioinizing radiation strikes the cloud
extinguish 24
#
# fix the temperature to 20 K =============
constant temperature 20
# stop at a radius of 4.3e-4 parsecs ============
stop thickness 0.00043 parsecs linear
# Le Petit model does not consider ices, so turn this off ============
no grain molecules
# turn on cosmic rays =========
cosmic rays background
# Set cosmic ray ionization rate to Table 2 of Le Petit paper ========
set csupra -15.6
# Allow calculation to go extend into cold environment ============
stop temperature linear 3
#
# commands controlling output ============
save performance "pdr_dense_persei.per"
save overview "pdr_dense_persei.ovr"
save dr "pdr_dense_persei.dr"
save molecules "pdr_dense_persei.mol"
save heating "pdr_dense_persei.het"
save cooling "pdr_dense_persei.col"
#
# pdr_dense_persei.in
# class pdr
# ==================================
```

This is the dense phase model presented by LePetit, Roueff, and Herbst in order to reproduce C2 and C3 column densities observed along the line of sight to zera persei. This is our attempt at reproducing their calculation. This is the dense molecular phase, not the phase that produces H3+

>>refer model pdr Le Petit, F., Roueff, E., & Herbst, E. 2004, # >>refercon A&A, 417, 993

If you do a thermal equilibrium calculation by removing the constant temperature command the kinetic temperature will be about three times larger than assumed in their paper.

---

pdr_HTT91.in

low-density PDR from HTT91

```
title low-density PDR from HTT91
# >>refer test model Hollenbach, D., Takahashi, T., &
# >>refcon Tielens, A.G.G.M., 1991, ApJ,377, 192-209
#
# commands controlling continuum =========
# first continuum is FIR hot grain continuum produced in
# unmodeled HII Region
```

```
# this is hot star continuum
black 30000
intensity 0.2 range 0.4412 to 1 Ryd
# this will remove all ionizing radiation
extinguish 24 0
cosmic rays, background
#
# commands for density & abundances =========
hden 3
init file="ism.ini"
abundances he= -1.01 c= -3.52 n=-8 o=-3.30 ne=-8 mg=-5.89
continue si= -6.10 s= -5.10 cl=-7 ar=-8 fe= -6.60
grains orion, abundance log 0.16 no qheat
#
# commands controlling geometry =========
sphere
# stop when gas is fully neutral
stop efrac -10
# this is to stop at an intended place, since results would be
# very dependent on details if we stop on temperature
stop thickness 18.954
# stop when gas is cold
stop temperature 10 linear
# add this to mimic unmodelled neutral gas
double optical depths
#
# other commands for details =========
iterate 2
Database H-like Lyman pumping off
turbulence 1.5 km/sec
#
# commands controlling output =========
normalize to "C 2" 157.636m
# uv lines are strongly pumped by stellar continuum, break out contribution
print line pump
print line optical depths
print ages
save performance "pdr_HTT91.per"
save overview last "pdr_HTT91.ovr"
save dr "pdr_HTT91.dr"
save molecules last "pdr_HTT91.mol"
save results last "pdr_HTT91.rlt"
save continuum units microns last "pdr_HTT91.con"
save heating last "pdr_HTT91.het"
save cooling last "pdr_HTT91.col"
#
# pdr_HTT91.in
# class pdr
# ======================================
#
```

This is the Hollenbach et al 1991 Low-density PDR The Database H-like Lyman pumping off command appears because the Lyman lines are vastly optically thick in this environment. If the command is removed the Lyman lines will be optically thin, which will result in fast fluorescent excitation of the (nearly totally neutral) hydrogen atom.

there is very little CO in this model since it is not thick enough for the UV pumping lines to become optically thick

---

pdr_leiden_f1.in

Leiden meeting model 1

```
title Leiden meeting model 1
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
```

```
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 5
extinguish 24
#
# commands for density & abundances =========
# hydrogen density
hden 3.
grains ism 1.16 no qheat
#
# commands controlling geometry =========
#
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden.ini"
# This command defines the grain temperature to be a constant 20 Kelvin
constant grain temperature 20
# This sets the temperature to a constant 50 Kelvin
constant temperature 50 linear
#
# commands controlling output =========
print line optical depths
save performance "pdr_leiden_f1.per"
save overview "pdr_leiden_f1.ovr"
save continuum "pdr_leiden_f1.con"
save leiden lines "pdr_leiden_f1.lin"
save leiden "pdr_leiden_f1.lei"
save dr "pdr_leiden_f1.dr"
save molecules "pdr_leiden_f1.mol"
save grain physical conditions "pdr_leiden_f1.grn"
save chemistry rates "pdr_leiden_f1.COr" "CO"
save chemistry rates "pdr_leiden_f1.H2r" "H2"
save chemistry rates "pdr_leiden_f1.H2a" "H2" all
save chemistry rates "pdr_leiden_f1.H2ds" "H2" destruction
save chemistry rates "pdr_leiden_f1.H2cr" "H2" creation
save chemistry rates "pdr_leiden_f1.H2ca" "H2" catalytic
save secondaries "pdr_leiden_f1.sec"
save species column densities "pdr_leiden_f1.col" all
#
#
#
# pdr_leiden_f1.in
# class pdr
# ======================================
#
```

This sim has some interesting properties. The grain temp is so low that O freezes onto grains as H2O. This is so efficient that CO does not become well formed - the CO/C ratio only reaches 0.3. This is one of the tests in Rollig et al. 2007, A&A, 467, 187

---

pdr_leiden_f2.in

Leiden meeting model 2

```
title Leiden meeting model 2
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use
# half the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 50000
extinguish 24
```

```
#
# commands for density & abundances =========
grains ism 1.16 no qheat
# hydrogen density
hden 3.
#
# commands controlling geometry =========
#
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden.ini"
# This command defines the grain temperature to be a constant 20 Kelvin
constant grain temperature 20
# This sets the temperature to a constant 50 Kelvin
constant temperature 50 linear
#
# commands controlling output =========
save performance "pdr_leiden_f2.per"
save overview "pdr_leiden_f2.ovr"
save continuum "pdr_leiden_f2.con"
save molecules "pdr_leiden_f2.mol"
save chemistry rates "pdr_leiden_f2.rat" "SiO"
save leiden lines "pdr_leiden_f2.lin"
save leiden "pdr_leiden_f2.lei"
save dr "pdr_leiden_f2.dr"
save grain physical conditions "pdr_leiden_f2.grn"
#
#
# pdr_leiden_f2.in
# class pdr
# ========================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187

---

pdr_leiden_f3.in

Leiden meeting model 3

```
title Leiden meeting model 3
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 5
extinguish 24
#
# commands for density & abundances =========
grains ism 1.16 no qheat
# hydrogen density
hden 5.5
#
# commands controlling geometry =========
#
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden.ini"
# This command defines the grain temperature to be a constant 20 Kelvin
constant grain temperature 20
# This sets the temperature to a constant 50 Kelvin
constant temperature 50 linear
```

```
#
# commands controlling output =========
save performance "pdr_leiden_f3.per"
save overview "pdr_leiden_f3.ovr"
save continuum "pdr_leiden_f3.con"
save leiden lines "pdr_leiden_f3.lin"
save leiden "pdr_leiden_f3.lei"
save dr "pdr_leiden_f3.dr"
save grain physical conditions "pdr_leiden_f3.grn"
#
#
# pdr_leiden_f3.in
# class pdr
# ======================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187

---

pdr_leiden_f4.in

Leiden meeting model 4

```
title Leiden meeting model 4
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
#
# commands for density & abundances =========
grains ism 1.16 no qheat
#
# commands controlling geometry =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 50000
extinguish 24
#
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden.ini"
# This command defines the grain temperature to be a constant 20 Kelvin
constant grain temperature 20
# This sets the temperature to a constant 50 Kelvin
constant temperature 50 linear
# hydrogen density
hden 5.5
#
# commands controlling output =========
save performance "pdr_leiden_f4.per"
save overview "pdr_leiden_f4.ovr"
save continuum "pdr_leiden_f4.con"
save leiden lines "pdr_leiden_f4.lin"
save leiden "pdr_leiden_f4.lei"
save dr "pdr_leiden_f4.dr"
save grain physical conditions "pdr_leiden_f4.grn"
#
#
# pdr_leiden_f4.in
# class pdr
# ======================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187

---

pdr_leiden_hack_f1.in

Leiden meeting model 1 with hacks

```
title Leiden meeting model 1 with hacks
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 5
extinguish 24
#
# commands for density & abundances =========
# hydrogen density
hden 3.
grains ism 1.16 no qheat
#
# commands controlling geometry =========
#
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden_hack.ini"
# This command defines the grain temperature to be a constant 20 Kelvin
constant grain temperature 20
# This sets the temperature to a constant 50 Kelvin
constant temperature 50 linear
#
# commands controlling output =========
save performance "pdr_leiden_hack_f1.per"
save leiden lines "pdr_leiden_hack_f1.lin"
save leiden "pdr_leiden_hack_f1.lei"
save dr "pdr_leiden_hack_f1.dr"
save grain physical conditions "pdr_leiden_hack_f1.grn"
save overview "pdr_leiden_hack_f1.ovr"
#
#
#
# class pdr
# ======================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187 this includes hacks to get "standard answer"

---

pdr_leiden_hack_f2.in

Leiden meeting model 2 with hacks

```
title Leiden meeting model 2 with hacks
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use
# half the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 50000
extinguish 24
#
# commands for density & abundances =========
grains ism 1.16 no qheat
# hydrogen density
```

```
hden 3.
#
# commands controlling geometry =========
#
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden_hack.ini"
# This command defines the grain temperature to be a constant 20 Kelvin
constant grain temperature 20
# This sets the temperature to a constant 50 Kelvin
constant temperature 50 linear
#
# commands controlling output =========
save performance "pdr_leiden_hack_f2.per"
save leiden lines "pdr_leiden_hack_f2.lin"
save leiden "pdr_leiden_hack_f2.lei"
save dr "pdr_leiden_hack_f2.dr"
save grain physical conditions "pdr_leiden_hack_f2.grn"
save overview "pdr_leiden_hack_f2.ovr"
#
#
# pdr_leiden_hack_f2.in
# class pdr
# ======================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187 includes hacks to get standard answer.

---

pdr_leiden_hack_f3.in

Leiden meeting model 3 with hacks

```
title Leiden meeting model 3 with hacks
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 5
extinguish 24
#
# commands for density & abundances =========
grains ism 1.16 no qheat
# hydrogen density
hden 5.5
#
# commands controlling geometry =========
#
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden_hack.ini"
# This command defines the grain temperature to be a constant 20 Kelvin
constant grain temperature 20
# This sets the temperature to a constant 50 Kelvin
constant temperature 50 linear
#
# commands controlling output =========
save performance "pdr_leiden_hack_f3.per"
save leiden lines "pdr_leiden_hack_f3.lin"
save overview "pdr_leiden_hack_f3.ovr"
save leiden "pdr_leiden_hack_f3.lei"
save dr "pdr_leiden_hack_f3.dr"
```

```
save grain physical conditions "pdr_leiden_hack_f3.grn"
#
#
# pdr_leiden_hack_f3.in
# class pdr
# ======================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187 include hacks to get standard answer.

---

pdr_leiden_hack_f4.in

Leiden meeting model 4 with hacks

```
title Leiden meeting model 4 with hacks
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
#
# commands for density & abundances =========
grains ism 1.16 no qheat
#
# commands controlling geometry =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 50000
extinguish 24
#
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden_hack.ini"
# This command defines the grain temperature to be a constant 20 Kelvin
constant grain temperature 20
# This sets the temperature to a constant 50 Kelvin
constant temperature 50 linear
# hydrogen density
hden 5.5
#
# commands controlling output =========
save performance "pdr_leiden_hack_f4.per"
save leiden lines "pdr_leiden_hack_f4.lin"
save leiden "pdr_leiden_hack_f4.lei"
save dr "pdr_leiden_hack_f4.dr"
save grain physical conditions "pdr_leiden_hack_f4.grn"
save overview "pdr_leiden_hack_f4.ovr"
#
#
# pdr_leiden_hack_f4.in
# class pdr
# ======================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187 includes hacks needed to get standard answer.

---

pdr_leiden_hack_v1.in

Leiden meeting model 5 with hacks

```
title Leiden meeting model 5 with hacks
```

```
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# is half the requested value
# they want for the model is actually twice the value below
table draine 5
extinguish 24
#
# commands for density & abundances =========
# hydrogen density
hden 3.
grains ism 1.16 no qheat
#
# commands controlling geometry =========
#
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden_hack.ini"
# Define the abundance of PAHs so we can reproduce the same photoelectric
# heating curve as BT94
# We have also scaled the grain abundance to achieve the desired AV/NH ratio
#
# commands controlling output =========
save performance "pdr_leiden_hack_v1.per"
save leiden lines "pdr_leiden_hack_v1.lin"
save leiden "pdr_leiden_hack_v1.lei"
save dr "pdr_leiden_hack_v1.dr"
save grain temperature "pdr_leiden_hack_v1.grn"
save overview "pdr_leiden_hack_v1.ovr"
#
#
# pdr_leiden_hack_v1.in
# class pdr
# ======================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187 includes hacks to get standard answer.

---

pdr_leiden_hack_v2.in

Leiden meeting model 6 with hacks

```
title Leiden meeting model 6 with hacks
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 50000
extinguish 24
#
# commands for density & abundances =========
# Define the abundance of PAHs so we can reproduce the same photoelectric
# heating curve as BT94
# We have also scaled the grain abundance to achieve the desired AV/NH ratio
grains ism 1.16 no qheat
# hydrogen density
hden 3.
#
# commands controlling geometry =========
#
```

```
# other commands for details =========
# use leiden initialization file
init file="pdr_leiden_hack.ini"
#
# commands controlling output =========
save performance "pdr_leiden_hack_v2.per"
save leiden lines "pdr_leiden_hack_v2.lin"
save leiden "pdr_leiden_hack_v2.lei"
save dr "pdr_leiden_hack_v2.dr"
save grain temperature "pdr_leiden_hack_v2.grn"
save overview "pdr_leiden_hack_v2.ovr"
save heating "pdr_leiden_hack_v2.het"
save cooling "pdr_leiden_hack_v2.col"
save h2 rates "pdr_leiden_hack_v2.h2rat"
#
#
# pdr_leiden_hack_v2.in
# class pdr
# ======================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187 includes hacks to get standard answer.

---

pdr_leiden_hack_v3.in

Leiden meeting model 7 with hacks

```
title Leiden meeting model 7 with hacks
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 5
extinguish 24
#
# commands for density & abundances =========
# Define the abundance of PAHs so we can reproduce the same photoelectric
# heating curve as BT94
# We have also scaled the grain abundance to achieve the desired AV/NH ratio
grains ism 1.16 no qheat
# hydrogen density
hden 5.5
#
# commands controlling geometry =========
#
# other commands for details =========
# this sim has more than one thermal solution - force into lowest one,
# the one found by the rest of the group - without this we will find a
# soln at 1400 K
force temperature to 60K
failures 3
# use leiden initialization file
init file="pdr_leiden_hack.ini"
#
# commands controlling output =========
save performance "pdr_leiden_hack_v3.per"
save leiden lines "pdr_leiden_hack_v3.lin"
save leiden "pdr_leiden_hack_v3.lei"
save dr "pdr_leiden_hack_v3.dr"
save grain temperature "pdr_leiden_hack_v3.grn"
save overview "pdr_leiden_hack_v3.ovr"
save heating "pdr_leiden_hack_v3.het"
save cooling "pdr_leiden_hack_v3.col"
```

```
#
#
# pdr_leiden_hack_v3.in
# class pdr
# ======================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187 includes hacks to get standard answer

---

pdr_leiden_hack_v4.in

Leiden meeting model 8 with hacks

```
title Leiden meeting model 8 with hacks
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 50000
extinguish 24
#
# commands for density & abundances =========
# Define the abundance of PAHs so we can reproduce the same photoelectric
# heating curve as BT94
# We have also scaled the grain abundance to achieve the desired AV/NH ratio
grains ism 1.16 no qheat
set PAH Bakes
# hydrogen density
hden 5.5
#
# commands controlling geometry =========
#
# other commands for details =========
# use leiden initialization file
init file="pdr_leiden_hack.ini"
#
# commands controlling output =========
save performance "pdr_leiden_hack_v4.per"
save leiden lines "pdr_leiden_hack_v4.lin"
save leiden "pdr_leiden_hack_v4.lei"
save dr "pdr_leiden_hack_v4.dr"
save grain temperature "pdr_leiden_hack_v4.grn"
save overview "pdr_leiden_hack_v4.ovr"
save heating "pdr_leiden_hack_v4.het"
save cooling "pdr_leiden_hack_v4.col"
save transmitted continuum "pdr_leiden_hack_v4.con"
#
#
# pdr_leiden_hack_v4.in
# class pdr
# ======================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187 includes hacks to get standard answer.

---

pdr_leiden_v1.in

Leiden meeting model 5

```
title Leiden meeting model 5
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# is half the requested value
# they want for the model is actually twice the value below
table draine 5
extinguish 24
#
# commands for density & abundances =========
# hydrogen density
hden 3.
grains ism 1.16 no qheat
# add PAHs
grains PAH no qheat 3 function
#
# commands controlling geometry =========
#
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden.ini"
#
# commands controlling output =========
save performance "pdr_leiden_v1.per"
save overview "pdr_leiden_v1.ovr"
save leiden lines "pdr_leiden_v1.lin"
save leiden "pdr_leiden_v1.lei"
save dr "pdr_leiden_v1.dr"
save grain temperature "pdr_leiden_v1.grn"
#
#
#
# pdr_leiden_v1.in
# class pdr
# ======================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187

---

pdr_leiden_v2.in

Leiden meeting model 6

```
title Leiden meeting model 6
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 50000
extinguish 24
#
# commands for density & abundances =========
# add PAHs and grains
grains PAH no qheat 3 function
grains ism 1.16 no qheat
# hydrogen density
hden 3.
#
# commands controlling geometry =========
```

```
#
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden.ini"
#
# commands controlling output =========
save performance "pdr_leiden_v2.per"
save overview "pdr_leiden_v2.ovr"
save leiden lines "pdr_leiden_v2.lin"
save leiden "pdr_leiden_v2.lei"
save dr "pdr_leiden_v2.dr"
save grain temperature "pdr_leiden_v2.grn"
#
#
# pdr_leiden_v2.in
# class pdr
# ======================================
#
```

This is one of the tests in Rollig et al. 2007, A&A, 467, 187

---

pdr_leiden_v3.in

Leiden meeting model 7

```
title Leiden meeting model 7
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 5
extinguish 24
#
# commands for density & abundances =========
# add PAHs and grains
grains PAH no qheat 3 function
grains ism 1.16 no qheat
# hydrogen density
hden 5.5
#
# commands controlling geometry =========
#
# other commands for details =========
failures 3
# use leiden initialization file
init file="pdr_leiden.ini"
#
# commands controlling output =========
save performance "pdr_leiden_v3.per"
save overview "pdr_leiden_v3.ovr"
save leiden lines "pdr_leiden_v3.lin"
save leiden "pdr_leiden_v3.lei"
save dr "pdr_leiden_v3.dr"
save grain temperature "pdr_leiden_v3.grn"
save heating "pdr_leiden_v3.het"
save cooling "pdr_leiden_v3.col"
#
#
# pdr_leiden_v3.in
# class pdr
# ======================================
#
```

pdr_leiden_v4.in

Leiden meeting model 8

```
title Leiden meeting model 8
# This is one of the tests in Rollig et al. 2007, A&A, 467, 187
#
# commands controlling continuum =========
# Use the Draine 1978 field, for a semi-infinite slab we have to use half
# the requested value, so the actual value
# they want for the model is actually twice the value below
table draine 50000
extinguish 24
#
# commands for density & abundances =========
grains PAH no qheat 3 function
grains ism 1.16 no qheat
# hydrogen density
hden 5.5
#
# commands controlling geometry =========
#
# other commands for details =========
# failures 3
# use leiden initialization file
init file="pdr_leiden.ini"
#
# commands controlling output =========
save performance "pdr_leiden_v4.per"
save overview "pdr_leiden_v4.ovr"
save leiden lines "pdr_leiden_v4.lin"
save leiden "pdr_leiden_v4.lei"
save dr "pdr_leiden_v4.dr"
save grain temperature "pdr_leiden_v4.grn"
save transmitted continuum "pdr_leiden_v4.con"
save heating "pdr_leiden_v4.het"
save cooling "pdr_leiden_v4.col"
#
#
# pdr_leiden_v4.in
# class pdr
# ======================================
#
```

---

pdr_minimal.in

test physical conditions at the illuminated face of a PDR

```
title test physical conditions at the illuminated face of a PDR
#
# commands controlling continuum =========
table draine 50000
extinguish 24
#
# commands for density & abundances =========
hden 5.5
element helium abundance -1.00
element lithium off
element beryllium off
element boron off
element carbon off
element oxygen off
```

```
element fluorine off
element neon off
element sodium off
element magnesium off
element aluminum off
element silicon off
element phosphorus off
element sulphur off
element chlorine off
element argon off
element potassium off
element calcium off
element scandium off
element titanium off
element vanadium off
element chromium off
element manganese off
element iron off
element cobalt off
element nickel off
element copper off
element zinc off
#
# other commands for details =========
constant temperature 50 linear
set dr 1
stop zone 2
stop temperature off
#
# commands controlling output =========
set save prefix "pdr_minimal"
save performance ".per" last
save overview ".ovr" last
save molecules ".mol" last
save leiden ".lei" last
save leiden lines ".lin" last
#
#
# IF EITHER OF THESE MONITORS NEEDS TO BE ADJUSTED, CHECK THAT THE IONIZATION
# CONDITIONS IN ZONE 1 AND 2 ARE IN VERY GOOD AGREEMENT!
#
# pdr_minimal.in
# class pdr
# ======================================
```

This model is derived from the F4 model from the Leiden workshop (Roellig et al. 2007, A&A, 467, 187). It has been reduced to a two-zone model in order to test the ionization conditions at the face of the PDR. Older versions of the code had a bug where the ionization in zone 1 was many dex lower than in zone 2. The conditions in zone 1 were wrong and should have been similar to the conditions in zone 2. Here we test that the code doesn't regress. See also ticket #358: https://wiki.nublado.org/ticket/358

The ionization in this sim is produced by continuum pumping of the metastable levels of N I, followed by photoionization out of the metastable levels of N I. See Ferland et al., 2012, ApJ, 757, 79. So this pumping and ionization mechanism is also tested by this sim.

---

pdr_orion_veil.in

Orion's veil

```
title Orion's veil
#
# commands controlling continuum =========
q(h) 50.000000
table SED "Rubin.sed"
```

```
# AGN & CMB background
background z=0
cosmic rays background
# as a test this was tried - atomic temperature raised fm 100 to 140
# but nothing really wrong
# the observed magnetic field, roughly 100 micro Gauss
magnetic field -4
#
# commands for density & abundances =========
hden 3.1
init "ism.ini"
element calcium on
abundances orion no grains
grains orion no qheat
element magnesium isotopes (24, 3) (25, 1) (26, 1)
#
# commands controlling geometry =========
stop neutral hydrogen column density 21.6
radius 19.1
stop temperature linear 5
# this will not be hit, but put it in to insure that we stop if
# gas becomes totally molecular
stop av 10
#
# other commands for details =========
failures 3
turbulence 0.5 km/sec
sphere
# c this simulates Lyman lines in the stellar continuum
# atom h-like lyman pumping off
#
# commands controlling output =========
print line optical depths
save overview "pdr_orion_veil.ovr"
save performance "pdr_orion_veil.per"
save PDR "pdr_orion_veil.pdr"
save species column densities "pdr_orion_veil.fe2col" "Fe+"
save hydrogen 21 cm "pdr_orion_veil.21cm"
save molecules "pdr_orion_veil.mol"
save overveiw "pdr_orion_veil.ovr"
save species column densities "pdr_orion_veil.cden" all
save heating "pdr_orion_veil.het"
save cooling "pdr_orion_veil.col"
save dr "pdr_orion_veil.dr"
save H2 rates "pdr_orion_veil.h2rat"
save pressure "pdr_orion_veil.pre"
save wind "pdr_orion_veil.wnd"
save continuum units microns "pdr_orion_veil.con" last
#
# pdr_orion_veil.in
# class pdr
# ======================================
#
```

This is Abel et al 2004 model of Orion's veil, the layer of gas in front of the Orion Nebula. >>refer Orion Veil Abel, N. P., Brogan, C. L., Ferland, G. J., >>refercon O'Dell, C. R., Shaw, G., & Troland, T. H. 2004

---

pdr_th85ism.in

TH85 PDR with ISM grains

```
title TH85 PDR with ISM grains
#
# commands controlling continuum =========
# cosmic radiation background
```

```
background z=0
# cosmic ray background ionization and heating
cosmic rays, background
# first continuum is FIR hot grain continuum produced in
# unmodeled HII Region
blackbody, t = 75 K
intensity 2.7 (total)
# this is the attenuated hot stellar continuum
black 30000
intensity 2.204 range 0.4412 to 1 Ryd
# this will remove all ionizing radiation
extinguish 24 0
#
# commands controlling geometry =========
# simulate effects of gas we do not model
double
# their turbulence
turbulence 2.7 km/sec
# stopping criteria
# this should be the one actually used
stop AV 33.2 extended
# stop when gas is fully neutral
stop efrac -10
# stop when gas is cold
stop temperature 10 linear
# stop at thickness of 16.5 so that mole limit does not
# stop this calculation - that would make results very
# detail dependent
stop thickness 19
#
# commands for density & abundances =========
hden 5.362
# this turns off some elements, and processes we don't need
# so needs to come before the elements
init file="ism.ini"
abundances he= -1.01 c= -3.52 n=-8 o=-3.30 ne=-8 mg=-5.89
continue si= -6.10 s= -5.10 cl=-7 ar=-8 fe= -6.60
# use ism abundances but turn of quantum heating
grains ism, abundance log 0.16 no qheat
#
# other commands for details =========
# must iterate since many FIR MIR lines are optically thick
iterate
# this is a closed geometry, in Orion, veil covers 2pi sr
sphere
# make Lyman lines very optically thick, which stops pumping by
# Balmer continuum
Database H-like Lyman pumping off
# this should run cleanly - turn down number of allow conv fails
failures 3
#
# commands controlling output =========
normalize to "c 2" 157.636m
# want the spectrum to be relative to this [C II] line
# uv lines are strongly pumped by stellar continuum, break out contribution
print line pump
print line optical depths
print ages
save performance "pdr_th85ism.per"
save overview last "pdr_th85ism.ovr"
save pdr last "pdr_th85ism.pdr"
save molecules last "pdr_th85ism.mol"
save dr last "pdr_th85ism.dr"
save hydrogen physical conditions last "pdr_th85ism.hyd"
save results last "pdr_th85ism.rlt"
save continuum units microns last "pdr_th85ism.con"
save heating last "pdr_th85ism.het"
save cooling last "pdr_th85ism.col"
save hydrogen 21 cm last "pdr_th85ism.21cm"
save element magnesium last "pdr_th85ism.mag"
```

```
save species levels "pdr_th85ism.lev" all
save species densities "pdr_th85ism.popCp" "C+[:]"
save species column density "pdr_th85ism.pop" "CO[:]"
save species densities "pdr_th85ism.poplist"
"*AV"
"*temp"
"e-"
C+
"C+[1:3]"
"CO[1]"
"CO[2]"
"H[1]"
"H[2]"
"He[1]"
"He[2]"
"He+[1]"
"He+[2]"
end of species
save grain extinction last "pdr_th85ism.grnext"
save grain potential last "pdr_th85ism.grnpot"
save grain temperature last "pdr_th85ism.grntem"
save grain charge last "pdr_th85ism.grnchr"
#
# pdr_th85ism.in
# class pdr
# ======================================
#
```

This is the Tielens and Hollenbach (1985a, b) standard model of the Orion photodissociation region (PDR). Specifically, this is my attempt at their Table 2 of paper 2, ApJ 291, p749. The Database H-like Lyman pumping off command appears because the Lyman lines are vastly optically thick in this environment. If the command is removed the Lyman lines will be optically thin, which will result in fast fluorescent excitation of the (nearly totally neutral) hydrogen atom.

>>refer model pdr Tielens, A. G. G. M., & Hollenbach, D. 1985a, ApJ, 291, 722 # >>refer model pdr Tielens, A. G. G. M., & Hollenbach, D. 1985b, ApJ, 291, 746

---

pdr_th85ism_cgto.in

TH85 pdr with ISM grains and C > O

```
title TH85 pdr with ISM grains and C > O
#
# commands controlling continuum =========
# cosmic radiation background
background z=0
# cosmic ray background ionization and heating
cosmic rays, background
# first continuum is FIR hot grain continuum produced in
# unmodeled HII Region
blackbody, t = 75 K
intensity 2.7 (total)
# this is the attenuated hot stellar continuum
black 30000
intensity 2.204 range 0.4412 to 1 Ryd
# this will remove all ionizing radiation
extinguish 24 0
#
# commands controlling geometry =========
# simulate effects of gas we do not model
double
# their turbulence
turbulence 2.7 km/sec
# stopping criteria
# this should be the one actually used
```

```
stop AV 33.2 extended
# stop when gas is fully neutral
stop efrac -10
# stop when gas is cold
stop temperature 10 linear
# stop at thickness of 16.5 so that mole limit does not
# stop this calculation - that would make results very
# detail dependent
stop thickness 19
#
# commands for density & abundances =========
hden 5.362
# this turns off some elements, and processes we don't need
# so needs to come before the elements
init file="ism.ini"
# this is the TH85 mix except C is raised by 0.2 dex,
# and O lowered byt his amount, so that C/O > 1
abundances he= -1.01 c= -3.4 n=-8 o=-3.50 ne=-8 mg=-5.89
continue si= -6.10 s= -5.10 cl=-7 ar=-8 fe= -6.60
# use ism abundances but turn of quantum heating
grains ism, abundance log 0.16 no qheat
#
# other commands for details =========
# must iterate since many FIR MIR lines are optically thick
iterate
# this is a closed geometry, in Orion, veil covers 2pi sr
sphere
# make Lyman lines very optically thick, which stops pumping by
# Balmer continuum
Database H-like Lyman pumping off
# this should run cleanly - turn down number of allow conv fails
failures 3
#
# commands controlling output =========
normalize to "c 2" 157.636m
# want the spectrum to be relative to this [C II] line
# uv lines are strongly pumped by stellar continuum, break out contribution
print line pump
print line optical depths
print ages
save performance "pdr_th85ism_cgto.per"
save overview last "pdr_th85ism_cgto.ovr"
save pdr last "pdr_th85ism_cgto.pdr"
save molecules last "pdr_th85ism_cgto.mol"
save dr last "pdr_th85ism_cgto.dr"
save hydrogen physical conditions last "pdr_th85ism_cgto.hyd"
save results last "pdr_th85ism_cgto.rlt"
save continuum units microns last "pdr_th85ism_cgto.con"
save heating last "pdr_th85ism_cgto.het"
save cooling last "pdr_th85ism_cgto.col"
save hydrogen 21 cm last "pdr_th85ism_cgto.21cm"
save element magnesium last "pdr_th85ism_cgto.mag"
save grain extinction last "pdr_th85ism_cgto.grnext"
save grain potential last "pdr_th85ism_cgto.grnpot"
save grain temperature last "pdr_th85ism_cgto.grntem"
save grain charge last "pdr_th85ism_cgto.grnchr"
#
# pdr_th85ism_cgto.in
# class pdr
# ========================================
#
```

This is the Tielens and Hollenbach (1985a, b) standard model of the Orion photodissociation region (PDR) but with the C abundance increased by 0.2 dex, and O lowered by this amount, so that C/O>1. Specifically, this is their Table 2 of paper 2, ApJ 291, p749. The Database H-like Lyman pumping off command appears because the Lyman lines are vastly optically thick in this environment. If the command is removed the Lyman lines will be optically thin, which will result in fast fluorescent excitation of the (nearly totally neutral) hydrogen atom.

>>refer model pdr Tielens, A. G. G. M., & Hollenbach, D. 1985a, ApJ, 291, 722 # >>refer model pdr Tielens, A. G. G. M., & Hollenbach, D. 1985b, ApJ, 291, 746

---

pdr_th85orion.in

TH85 PDR with Orion grains

```
title TH85 PDR with Orion grains
#
# commands controlling continuum =========
# cosmic background
background
# galactic cosmic ray background
cosmic rays, background
# first continuum is FIR hot grain continuum produced in
# unmodeled HII Region
blackbody, t = 75 K
intensity 2.7 (total)
# this is the attenuated hot stellar continuum
black 30000
intensity 2.204 range 0.4412 to 1 Ryd
# this will remove all ionizing radiation
extinguish 24 0
#
# commands for density & abundances =========
hden 5.362
init file="ism.ini"
grains orion, abundance log 0.16 no qheat
abundances he=-1.01 c=-3.52 n=-8 o=-3.30 ne=-8 mg=-5.89
continue si= -6.10 s= -5.10 cl=-7 ar=-8 fe= -6.60
#
# commands controlling geometry =========
# simulate effects of gas we do not model
double
sphere
# stopping criteria
# this should be the one actually used
# >>chn 04 mar 13, from 10 to 36.3, bug in AV had stopped at this depth,
# so change it to this to keep model the same
stop AV 36.3 extended
# stop when gas is fully neutral
stop efrac -10
# stop when gas is cold
stop temperature 10 linear
# stop at thickness so that would make results very
# detail dependent
stop thickness 19
#
# other commands for details =========
turbulence 2.7 km/sec
iterate
failures 3
#
# this is done to not allow pumping and subsequent photoionization
# of H by Balmer continuum in keeping with std pdr assumptions
Database H-like Lyman pumping off
#
# commands controlling output =========
normalize to "c 2" 157.636m
# uv lines are strongly pumped by stellar continuum, break out contribution
print line pump
print line optical depths
print ages
#
save performance "pdr_th85orion.per"
```

```
save overview "pdr_th85orion.ovr"
save pdr last "pdr_th85orion.pdr"
# this only outputs major molecules
save molecules last "pdr_th85orion.mol"
save dr "pdr_th85orion.dr"
# this is to get all of H molecules
save hydrogen physical conditions last "pdr_th85orion.hyd"
save results last "pdr_th85orion.rlt"
save continuum units microns last "pdr_th85orion.con"
save ionizing continuum last "pdr_th85orion.ion"
save heating last "pdr_th85orion.het"
save cooling last "pdr_th85orion.col"
save hydrogen 21 cm last "pdr_th85orion.21cm"
# these are for the grains
save grain extinction last "pdr_th85orion.grnext"
save grain potential last "pdr_th85orion.grnpot"
save grain temperature last "pdr_th85orion.grntem"
save grain charge last "pdr_th85orion.grnchr"
#
#
# pdr_th85orion.in
# class pdr
# ======================================
```

This is the Tielens and Hollenbach (1985a, b) standard model of the Orion photodissociation region (PDR). Specifically, this is my attempt at their Table 2 of paper 2, ApJ 291, p749. The Database H-like Lyman pumping off command appears because the Lyman lines are vastly optically thick in this environment. If the command is removed the Lyman lines will be optically thin, which will result in fast fluorescent excitation of the (nearly totally neutral) hydrogen atom.

>>refer model pdr Tielens, A. G. G. M., & Hollenbach, D. 1985a, ApJ, 291, 722 # >>refer model pdr Tielens, A. G. G. M., & Hollenbach, D. 1985b, ApJ, 291, 746

---

pn_fluc.in

Paris PN with density fluctuations

```
title Paris PN with density fluctuations
set save prefix "pn_fluc"
#
# commands for density & abundances =========
fluctuations 16.5 4 3
# this sets up the code like version c84, with fewer chemical elements
init file="c84.ini"
# this sets the abundances of the elements that we will use
abund He=-1 C=-3.523 N=-4. O=-3.222 ne=-3.824 na=-10 mg=-4.523 al=-10
continue si=-4.523 s=-4.824 ar=-10 ca=-10 fe=-10 ni=-10
#
# commands controlling continuum =========
black body, T = 150000 K, radius = 10
black 5
luminosity total 38
#
# commands controlling geometry =========
sphere
radius 17
#
# other commands for details =========
#
# commands controlling output =========
save performance ".per"
save overview last ".ovr"
save element nitrogen last ".nit"
save dr last ".dr"
save results last ".rlt"
```

```
#
# pn_fluc.in
# class pn function
# ======================================
```

The boundary conditions are similar to those for the Paris meeting PN, a homogeneous grain-free PN. This model has density fluctuations, with values chosen so that the mean ne np V are the same for the nebulae with and without fluctuations.

Checks:
- Check that the fluctuations command works.
- How do results compare with homogeneous Paris pn?

---

pn_ots.in

Paris PN with ots

```
title Paris PN with ots
# recompute "standard" PN model of the Pequignot Meudon Conference
#
# commands controlling continuum =========
black body, T = 150000 K, radius = 10
#
# commands for density & abundances =========
hden = 3.4771213
init file="c84.ini"
abund He=-1 C=-3.523 N=-4. O=-3.222 ne=-3.824 na=-10 mg=-4.523 al=-10
continue si=-4.523 s=-4.824 ar=-10 ca=-10 fe=-10 ni=-10
#
# commands controlling geometry =========
radius = 17
sphere
#
# other commands for details =========
diffuse ots
no level2
iterate
database h-like element hydrogen levels resolved 10
database h-like element helium levels resolved 15
#
# commands controlling output =========
save performance "pn_ots.per"
save overview last "pn_ots.ovr"
save element nitrogen last "pn_ots.nit"
save results last "pn_ots.rlt"
save dr last "pn_ots.dr"
#
# pn_ots.in
# class pn
# ======================================
#
```

This is the on-the-spot version of the Paris Planetary Nebula.
Checks:
- Q(H) total 4861 luminosity is close to expected value
- Line spectrum similar to that predicted by default conditions.

---

pn_paris.in

"Paris meeting PN"

```
title "Paris meeting PN"
set save prefix "pn_paris"
# standard" PN model of the Pequignot Meudon Conference
#
# commands controlling continuum =========
black body, T = 150000 K, radius = 10
#
# commands for density & abundances =========
hden = 3.4771213
init file="ism.ini"
# these elements were not part of the workshop models
element chlorine off
element argon off
element iron off
abund he=-1 C=-3.523 N=-4. O=-3.222 ne=-3.824 mg=-4.523
continue si=-4.523 s=-4.824 cl=-7 ar=-10 fe=-10
#
# commands controlling geometry =========
radius = 17
sphere
#
# other commands for details =========
age 10^2^2 years
#
# commands controlling output =========
print lines sort wavelength
normalize to "Ca b" 4861.32A
# the normalizing line is not defined on the emergent line stack
print lines emergent off
print line optical depths
print ages
print column densities
save performance ".per"
save overview ".ovr"
save transmitted continuum ".trn"
save continuum units microns ".con"
save element carbon ".car"
save physical conditions ".phy"
save element nitrogen ".nit"
save dr ".dr"
save temperature ".tem"
save lines emissivity ".ems"
h 1 6562.80A
Blnd 6720
end of lines
save averages ".avr" last
temperature hydrogen 1
end of averagers
#
# pn_paris.in
# class pn
# ======================================
#
```

This is one of the "standard" models computed at the Paris meeting on photoionization and shock calculations. A table in Hazy compares the predictions of the current version of CLOUDY with predictions of a few of the other codes.

The model is meant to represent a planetary nebula ionized by a very hot central object. As a result there is a great deal of He++ and the associated line and continuum emission is very important.

An age of 10000 years was set. This tests logic in the age command.

---

pn_paris_cpre.in

"Paris meeting PN with constant pressure"

```
title "Paris meeting PN with constant pressure"
# standard" PN model of the Pequignot Meudon Conference
#
# commands controlling continuum =========
black body, T = 150000 K, radius = 10
#
# commands for density & abundances =========
hden = 3.4771213
constant pressure
init file="ism.ini"
# these elements were not part of the workshop models
element chlorine off
element argon off
element iron off
abund he=-1 C=-3.523 N=-4. O=-3.222 ne=-3.824 mg=-4.523
continue si=-4.523 s=-4.824 cl=-7 ar=-10 fe=-10
#
# commands controlling geometry =========
radius = 17
sphere
#
# other commands for details =========
age 10^2^2 years
#
# commands controlling output =========
print lines sort wavelength
normalize to "Ca b" 4861.32A
# the normalizing line is not defined on the emergent line stack
print lines emergent off
print line optical depths
print ages
print column densities
save performance "pn_paris_cpre.per"
save overview "pn_paris_cpre.ovr"
save transmitted continuum "pn_paris_cpre.trn"
save continuum units microns "pn_paris_cpre.con"
save element carbon "pn_paris_cpre.car"
save physical conditions "pn_paris_cpre.phy"
save element nitrogen "pn_paris_cpre.nit"
save dr "pn_paris_cpre.dr"
save temperature "pn_paris_cpre.tem"
save lines emissivity "pn_paris_cpre.ems"
h 1 6562.80A
Blnd 6720
end of lines
save averages "pn_paris_cpre.avr" last
temperature hydrogen 1
end of averagers
#
# pn_paris_cpre.in
# class pn
# ======================================
#
```

This is one of the "standard" models computed at the Paris meeting on photoionization and shock calculations, modified by assuming constant pressure within the nebula.

---

pn_paris_fast.in

Paris PN, fast version

```
title Paris PN, fast version
# standard" PN model of the Pequignot Meudon Conference
#
```

```
# commands controlling continuum =========
black body, T = 150000 K, radius = 10
#
# commands for density & abundances =========
hden = 3.4771213
init file="fast.ini"
abund he=-1 C=-3.523 N=-4. O=-3.222 ne=-3.824 mg=-4.523
continue si=-4.523 s=-4.824 ar=-10
#
# commands controlling geometry =========
sphere
radius = 17
#
# other commands for details =========
#
# commands controlling output =========
normalize to "Ca b" 4861.32A
# the normalizing line is not defined on the emergent line stack
print lines emergent off
save performance "pn_paris_fast.per"
save overview "pn_paris_fast.ovr"
save physical conditions "pn_paris_fast.phy"
save element nitrogen "pn_paris_fast.nit"
save dr "pn_paris_fast.dr"
#
# pn_paris_fast.in
# class pn
# ======================================
#
```

This is one of the "standard" models computed at the Paris meeting on photoionization and shock calculations. A table in Hazy compares the predictions of the current version of CLOUDY with predictions of a few of the other codes.

The model is meant to represent a planetary nebula ionized by a very hot central object. As a result there is a great deal of He++ and the associated line and continuum emission is very important.

---

pn_sqrden.in

PN with density propt R^-2 and filling factor

```
title PN with density propt R^-2 and filling factor
# this is an optically thin model, which will have a broad range
# of density but the same ionization parameter across the model.
# the physical condtions should not vary by much across the structure
#
# commands controlling continuum =========
# continuum is hot blackbody at ~Ledd for solar mass
blackbody, t=5 luminosity=38
#
# commands for density & abundances =========
# the density will fall off as the inverse square of the radius, hence the name
hden 5 -2
init file "ism.ini"
# use default PN abundances but turn off quantum heating since
# we are not going to save the predicted near IR continuum
abundances planetary no qheat
#
# commands controlling geometry =========
# small filling factor so that region will be optically thin
filling factor -2
# set inner and outer radius
radius 16 18
sphere
#
# other commands for details =========
```

```
iterate
#
# commands controlling output =========
print line faint 1
save performance "pn_sqrden.per"
save overview "pn_sqrden.ovr" last
save dr "pn_sqrden.dr" last
save molecules "pn_sqrden.mol"
#
# pn_sqrden.in
# class pn
# ======================================
```

Checks:
- Zone thickness budgeting handled OK.
- physical conditions nearly constant across computed structure

---

rrc_o.in

he-like oxygen ion vs. Bautista & Kallman 2000 Table 1, column 3

```
title he-like oxygen ion vs. Bautista & Kallman 2000 Table 1, column 3
#
# commands controlling continuum =========
laser 100
ionization -1
#
# commands for density & abundances =========
hden 7
# include lots of the element we are testing and set the ionization
# to be dominated by the correct ion stage
element oxygen abundance -2.0458
element oxygen ionization -1 -1 -1 -1 -1 -1 -1 -1 -1
init file "ism.ini"
element helium off
element nitrogen off
element carbon off
element neon off
element magnesium off
element silicon off
element sulphur off
element argon off
element iron off
#
# commands controlling geometry =========
stop zone 1
set dr -12
#
# other commands for details =========
constant temper 5
iterate
#
# commands controlling output =========
print line faint -5
save overview "rrc_o.ovr"
save performance "rrc_o.per"
save continuum "rrc_o.con" units Angstroms last
# rrc_o.in
# class limit
# ======================================
#
```

test RRC of simple and iso model atoms. The ionization is set to 10% for all stages of ionization of O. We monitor the ground state recombination emission. This is an optically thin model.

---

stars_atlas.in

Atlas stellar atmosphere

```
title Atlas stellar atmosphere
#
# commands controlling continuum =========
# Approximate model of a hot star ionizing its surroundings.
# Assume H density of 1e+6 per cc. This run tests the new Kurucz model option.
# I choose the T_eff and log(g) values arbitrarily. It implies a star
# with luminosity 32300 L_sun, radius 6.4745 R_sun, and mass 3.745 M_sun.
table star atlas 30400.0 4.2
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -3.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature 4
no blends
#
# commands controlling output =========
#
save performance "stars_atlas.per"
save overview last "stars_atlas.ovr"
save results last "stars_atlas.rlt"
save transmitted continuum last "stars_atlas.trn" no header
save continuum last "stars_atlas.con" units angstrom
#
# stars_atlas.in
# class stars
# ======================================
```

This is a test that the code can correctly access the large block of Atlas model atmosphere continua described by Kurucz (1991). Kevin Volk provided it as part of his original coding of these stellar atmosphere files. Constant temperature is assumed since this tests shape of stellar continuum rather than thermal physics.

Checks: table star atlas command works.

---

stars_atlas_3d.in

Atlas stellar atmosphere, 3D interpolation

```
title Atlas stellar atmosphere, 3D interpolation
#
# commands controlling continuum =========
# Approximate model of a hot star ionizing its surroundings.
# Assume H density of 1e+6 per cc. This run tests the atlas 3dim model option.
```

```
# I choose the T_eff and log(g) values arbitrarily.
table star atlas 3-dim 38400.0 4.82 -1.42
luminosity 4.509202522 solar
table star atlas odfnew 3-dim 38400.0 4.82 0.42
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -3.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature 4
no blends
#
# commands controlling output =========
#
save performance "stars_atlas_3d.per"
save overview last "stars_atlas_3d.ovr"
save results last "stars_atlas_3d.rlt"
save transmitted continuum last "stars_atlas_3d.trn" no header
save continuum last "stars_atlas_3d.con" units angstrom
#
# stars_atlas_3d.in
# class stars
# ======================================
```

This is a test that the code can correctly access the large 3-dim block of Atlas model atmosphere continua.

Checks: table star atlas 3dim command works.

---

stars_atlas_all.in

interpolate on Atlas grids

```
title interpolate on Atlas grids
#
# commands controlling continuum =========
# Include stars with a wide range of metallicities to test access to these grids.
table star atlas Z+1.0 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z+0.5 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z+0.3 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z+0.2 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z+0.1 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z+0.0 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z-0.1 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z-0.2 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z-0.3 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z-0.5 38400.0 4.82
```

```
luminosity 4.509202522 solar
table star atlas Z-1.0 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z-1.5 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z-2.0 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z-2.5 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z-3.0 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z-3.5 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z-4.0 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z-4.5 38400.0 4.82
luminosity 4.509202522 solar
table star atlas Z-5.0 38400.0 4.82
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -2.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature 4
no blends
#
# commands controlling output =========
#
save performance "stars_atlas_all.per"
save overview last "stars_atlas_all.ovr"
save results last "stars_atlas_all.rlt"
save transmitted continuum last "stars_atlas_all.trn" no header
save continuum last "stars_atlas_all.con" units angstrom
#
# stars_atlas_all.in
# class stars
# ======================================
```

This is a test that the code can correctly access the 2D grids of various metallicity of Atlas model atmosphere continua.

Checks: access to the various atlas grids

---

stars_atlas_odfnew_all.in

access various Atlas ODFNEW grids

```
title access various Atlas ODFNEW grids
#
# commands controlling continuum =========
# Include stars with a wide range of metallicities to test access to these grids.
table star atlas odfnew Z+0.5 38400.0 4.82
luminosity 4.509202522 solar
table star atlas odfnew Z+0.2 38400.0 4.82
luminosity 4.509202522 solar
table star atlas odfnew Z+0.0 38400.0 4.82
```

```
luminosity 4.509202522 solar
table star atlas odfnew Z-0.5 38400.0 4.82
luminosity 4.509202522 solar
table star atlas odfnew Z-1.0 38400.0 4.82
luminosity 4.509202522 solar
table star atlas odfnew Z-1.5 38400.0 4.82
luminosity 4.509202522 solar
table star atlas odfnew Z-2.0 38400.0 4.82
luminosity 4.509202522 solar
table star atlas odfnew Z-2.5 38400.0 4.82
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -2.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature 4
no blends
#
# commands controlling output =========
#
save performance "stars_atlas_odfnew_all.per"
save overview last "stars_atlas_odfnew_all.ovr"
save results last "stars_atlas_odfnew_all.rlt"
save transmitted continuum last "stars_atlas_odfnew_all.trn" no header
save continuum last "stars_atlas_odfnew_all.con" units angstrom
#
# stars_atlas_odfnew_all.in
# class stars
# ======================================
```

This is a test that the code can correctly access the Atlas ODFNEW model atmosphere continua.

Checks: access to the various atlas odfnew grids

---

stars_bstar2006.in

tlusty bstar grid

```
title tlusty bstar grid
#
# commands controlling continuum =========
# Approximate model of a B star ionizing its surroundings.
# Assume H density of 1e+6 per cc. This run tests the new Tlusty model option.
# I choose the T_eff and log(g) values arbitrarily.
table star tlusty bstar 20400.0 4.2
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -3.0 parsec
sphere
```

```
stop zone 1
set dr 0
#
# other commands for details =========
#
# in this model the Lyman lines are pumped significantly by the stellar continuum;
# disable this process to avoid critical dependence on the precise shape of the continuum.
no induced processes
constant temperature 4
no blends
#
# commands controlling output =========
#
save performance "stars_bstar2006.per"
save overview last "stars_bstar2006.ovr"
save results last "stars_bstar2006.rlt"
save continuum last "stars_bstar2006.con" units angstrom
save transmitted continuum last "stars_bstar2006.trn" no header
#
# stars_bstar2006.in
# class stars
# ======================================
```

This is a test that the code can correctly access the large block of Tlusty B-star model atmosphere continua.

Checks: table star tlusty bstar command works.

---

stars_bstar2006_3d.in

tlusty bstar grid

```
title tlusty bstar grid
#
# commands controlling continuum =========
# Approximate model of a B star ionizing its surroundings.
# Assume H density of 1e+6 per cc. This run tests the new Tlusty model option.
# I choose the T_eff, log(g) and log(Z) values arbitrarily.
table star tlusty bstar 3-dim 20400.0 4.2 -0.573
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -3.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
#
# in this model the Lyman lines are pumped significantly by the stellar continuum;
# disable this process to avoid critical dependence on the precise shape of the continuum.
no induced processes
constant temperature 4
no blends
#
# commands controlling output =========
#
save performance "stars_bstar2006_3d.per"
save overview last "stars_bstar2006_3d.ovr"
save results last "stars_bstar2006_3d.rlt"
```

```
save continuum last "stars_bstar2006_3d.con" units angstrom
save transmitted continuum last "stars_bstar2006_3d.trn" no header
#
# stars_bstar2006_3d.in
# class stars
# ======================================
```

This is a test that the code can correctly access the large 3-dim block of Tlusty B-star model atmosphere continua.

Checks: table star tlusty bstar 3-dim command works.

---

stars_bstar2006_all.in

tlusty bstar grid

```
title tlusty bstar grid
#
# commands controlling continuum =========
# Approximate model of 6 B stars ionizing their surroundings.
# Assume H density of 1e+6 per cc. This run tests all the various
# metallicities contained in the BSTAR 2006 grids. I choose the T_eff
# and log(g) values arbitrarily.
table star tlusty bstar Z+0.3 20000.0 4.5
luminosity 4.509202522 solar
table star tlusty bstar Z+0.0 21400.0 4.5
luminosity 4.509202522 solar
table star tlusty bstar Z-0.3 15000.0 4.2
luminosity 4.509202522 solar
table star tlusty bstar Z-0.7 20400.0 4.2
luminosity 4.509202522 solar
table star tlusty bstar Z-1.0 27500.0 3.0
luminosity 4.509202522 solar
table star tlusty bstar Z-INF 18000.0 4.75
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -2.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
no blends
#
# in this model the Lyman lines are pumped significantly by the stellar continuum;
# disable this process to avoid critical dependence on the precise shape of the continuum.
no induced processes
constant temperature 4
#
# commands controlling output =========
#
save performance "stars_bstar2006_all.per"
save overview last "stars_bstar2006_all.ovr"
save results last "stars_bstar2006_all.rlt"
save continuum last "stars_bstar2006_all.trn" units angstrom
save transmitted continuum last "stars_bstar2006_all.trn" no header
#
# stars_bstar2006_all.in
```

```
# class stars
# ======================================
```

This is a test that the code can correctly access the large block of Tlusty B-star model atmosphere continua.

Checks: table star tlusty bstar metallicity option works.

---

stars_costar1.in

costar interpolation mode 1

```
title costar interpolation mode 1
#
# commands controlling continuum =========
table star costar, 40000 K
ionization parameter -2
table star costar, 31000 K, index 4
ionization parameter -2
#
# commands for density & abundances =========
hden 2
grains orion single no qheat
abundances ism no grains
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
constant temperature 6000K
no blends
#
# commands controlling output =========
save overview "stars_costar1.ovr"
save performance "stars_costar1.per"
save continuum last "stars_costar1.con" units angstrom
#
# stars_costar1.in
# class stars
# ======================================
#
```

This is a test of whether the code can read the CoStar stellar atmospheres. It checks the resulting ionization to confirm that the continuum shape was ok. Constant temperature is assumed since this tests shape of stellar continuum rather than thermal physics.

---

stars_costar2.in

costar interpolation mode 2

```
title costar interpolation mode 2
#
# commands controlling continuum =========
table star costar 35575.4 4.2367
ionization parameter -2
table star costar 34468.5 3.86765
ionization parameter -2
table star costar 41741.2 4.02
ionization parameter -2
```

```
table star costar 45000 4.1593
ionization parameter -2
table star costar 27500 3.3
ionization parameter -2
#
# commands for density & abundances =========
hden 2
grains orion single no qheat
abundances ism no grains
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
no blends
#
# commands controlling output =========
save overview "stars_costar2.ovr"
save performance "stars_costar2.per"
save continuum last "stars_costar2.con" units angstrom
#
# stars_costar2.in
# class stars
# ======================================
#
```

This is a test of whether the code can read the CoStar stellar atmospheres. It checks the resulting ionization to confirm that the continuum shape was ok.

---

stars_costar3.in

costar interpolation mode 3

```
title costar interpolation mode 3
#
# commands controlling continuum =========
table star costar zams 40.0 Msol 2.85e6
ionization parameter -2
table star costar zams 40.0 Msol 4e6
ionization parameter -2
table star costar zams 50.9 Msol 2.85e6
ionization parameter -2
table star costar zams 42.9 Msol 1.6e6
ionization parameter -2
table star costar zams 70.5 Msol 2.1e6
ionization parameter -2
#
# commands for density & abundances =========
hden 2
grains orion single no qheat
abundances ism no grains
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
no blends
#
# commands controlling output =========
save overview "stars_costar3.ovr"
save performance "stars_costar3.per"
save continuum last "stars_costar3.con" units angstrom
#
```

```
# stars_costar3.in
# class stars
# ======================================
#
```

This is a test of whether the code can read the CoStar stellar atmospheres. It checks the resulting ionization to confirm that the continuum shape was ok.

---

stars_costar4.in

costar interpolation mode 4

```
title costar interpolation mode 4
#
# commands controlling continuum =========
table star costar age 2.85e6 40.0
ionization parameter -2
table star costar age 4e6 40.0
ionization parameter -2
table star costar age 2.85e6 50.9
ionization parameter -2
table star costar age 1.6e6 42.9
ionization parameter -2
table star costar age 2.1e6 70.5
ionization parameter -2
#
# commands for density & abundances =========
hden 2
grains orion single no qheat
abundances ism no grains
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
no blends
#
# commands controlling output =========
save overview "stars_costar4.ovr"
save performance "stars_costar4.per"
save continuum last "stars_costar4.con" units angstrom
#
# stars_costar4.in
# class stars
# ======================================
#
```

This is a test of whether the code can read the CoStar stellar atmospheres. It checks the resulting ionization to confirm that the continuum shape was ok.

---

stars_costarhalo.in

costar halo abundances

```
title costar halo abundances
#
# commands controlling continuum =========
table star costar, halo abundances, 40000 K
ionization parameter -2
#
```

```
# commands for density & abundances =========
hden 2
abundances ism
#
# commands controlling geometry =========
set dr 0
stop zone 1
#
# other commands for details =========
constant temperature 6900K
no blends
#
# commands controlling output =========
save overview "stars_costarhalo.ovr"
save performance "stars_costarhalo.per"
save continuum last "stars_costarhalo.con" units angstrom
#
#
# stars_costarhalo.in
# class stars
# ======================================
#
```

This test checks that the code can read the CoStar stellar atmospheres. It checks the resulting ionization to make sure that the continuum shape is ok. Constant temperature is assumed since this tests shape of stellar continuum rather than thermal physics.

---

stars_kurucz79.in

Kurucz 1979 SED

```
title Kurucz 1979 SED
#
# commands controlling continuum =========
# Approximate model of a hot star ionizing its surroundings.
# Assume H density of 1e+6 per cc. This run tests the Kurucz model option.
# I choose the T_eff and log(g) values arbitrarily. It implies a star
# with luminosity 32300 L_sun, radius 6.4745 R_sun, and mass 3.745 M_sun.
table star kurucz 30400.0
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -3.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature 4
no blends
#
# commands controlling output =========
#
save performance "stars_kurucz79.per"
save overview last "stars_kurucz79.ovr"
save results last "stars_kurucz79.rlt"
save transmitted continuum last "stars_kurucz79.trn" no header
save continuum last "stars_kurucz79.con" units angstrom
#
# stars_kurucz79.in
```

```
# class stars
# ======================================
```

This is a test that the code can correctly access the Kurucz model atmosphere continua described by Kurucz (1979). Kevin Volk provided it as part of his original coding of these stellar atmosphere files. Constant temperature is assumed since this tests shape of stellar continuum rather than thermal physics.

Checks: table star kurucz command works.

---

stars_mihalas.in

Mihalas SED

```
title Mihalas SED
#
# commands controlling continuum =========
# Approximate model of a hot star ionizing its surroundings.
# Assume H density of 1e+6 per cc. This run tests the new Kurucz model option.
# I choose the T_eff and log(g) values arbitrarily. It implies a star
# with luminosity 32300 L_sun, radius 6.4745 R_sun, and mass 3.745 M_sun.
table star mihalas 30400.0
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -3.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
constant temperature 4
no blends
#
# commands controlling output =========
#
save performance "stars_mihalas.per"
save overview last "stars_mihalas.ovr"
save results last "stars_mihalas.rlt"
save transmitted continuum last "stars_mihalas.trn" no header
save continuum last "stars_mihalas.con" units angstrom
#
# stars_mihalas.in
# class stars
# ======================================
```

This is a test that the code can correctly access the small Mihalas grid of NLTE model atmospeheres Constant temperature is assumed since this tests shape of continuum not thermal physics.

Checks: table star mihalas command works.

---

stars_obstar_merged.in

tlusty bstar grid

```
title tlusty bstar grid
#
# commands controlling continuum =========
# Approximate model of a B star ionizing its surroundings.
# Assume H density of 1e+6 per cc. This run tests the new Tlusty model option.
# I choose the T_eff and log(g) values arbitrarily.
table star tlusty obstar 20400.0 4.2
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -3.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
no blends
#
# in this model the Lyman lines are pumped significantly by the stellar continuum;
# disable this process to avoid critical dependence on the precise shape of the continuum.
no induced processes
constant temperature 4
#
# commands controlling output =========
#
save performance "stars_obstar_merged.per"
save overview last "stars_obstar_merged.ovr"
save results last "stars_obstar_merged.rlt"
save continuum last "stars_obstar_merged.con" units angstrom
save transmitted continuum last "stars_obstar_merged.trn" no header
#
# stars_obstar_merged.in
# class stars
# ======================================
```

This is a test that the code can correctly access the large block of Tlusty B-star model atmosphere continua.

Checks: table star tlusty obstar command works.

---

stars_obstar_merged_3d.in

tlusty bstar grid

```
title tlusty bstar grid
#
# commands controlling continuum =========
# Approximate model of a B star ionizing its surroundings.
# Assume H density of 1e+6 per cc. This run tests the new Tlusty model option.
# I choose the T_eff, log(g) and log(Z) values arbitrarily.
table star tlusty obstar 3-dim 20400.0 4.2 -0.573
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
```

```
radius -3.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
#
# in this model the Lyman lines are pumped significantly by the stellar continuum;
# disable this process to avoid critical dependence on the precise shape of the continuum.
no induced processes
constant temperature 4
no blends
#
# commands controlling output =========
#
save performance "stars_obstar_merged_3d.per"
save overview last "stars_obstar_merged_3d.ovr"
save results last "stars_obstar_merged_3d.rlt"
save continuum last "stars_obstar_merged_3d.con" units angstrom
save transmitted continuum last "stars_obstar_merged_3d.trn" no header
#
# stars_obstar_merged_3d.in
# class stars
# ======================================
```

This is a test that the code can correctly access the large 3-dim block of Tlusty B-star model atmosphere continua.

Checks: table star tlusty obstar 3-dim command works.

---

stars_obstar_merged_all.in

tlusty bstar grid

```
title tlusty bstar grid
#
# commands controlling continuum =========
# Approximate model of 6 B stars ionizing their surroundings.
# Assume H density of 1e+6 per cc. This run tests all the various
# metallicities contained in the BSTAR 2006 grids. I choose the T_eff
# and log(g) values arbitrarily.
table star tlusty obstar Z+0.3 40000.0 4.5
luminosity 4.509202522 solar
table star tlusty obstar Z+0.0 21400.0 4.5
luminosity 4.509202522 solar
table star tlusty obstar Z-0.3 35000.0 4.2
luminosity 4.509202522 solar
table star tlusty obstar Z-0.7 20400.0 4.2
luminosity 4.509202522 solar
table star tlusty obstar Z-1.0 27500.0 3.0
luminosity 4.509202522 solar
table star tlusty obstar Z-INF 18000.0 4.75
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -2.0 parsec
sphere
stop zone 1
set dr 0
#
```

```
# other commands for details =========
#
# in this model the Lyman lines are pumped significantly by the stellar continuum;
# disable this process to avoid critical dependence on the precise shape of the continuum.
no induced processes
constant temperature 4
no blends
#
# commands controlling output =========
#
save performance "stars_obstar_merged_all.per"
save overview last "stars_obstar_merged_all.ovr"
save results last "stars_obstar_merged_all.rlt"
save continuum last "stars_obstar_merged_all.trn" units angstrom
save transmitted continuum last "stars_obstar_merged_all.trn" no header
#
# stars_obstar_merged_all.in
# class stars
# ======================================
```

This is a test that the code can correctly access the large block of Tlusty B-star model atmosphere continua.

Checks: table star tlusty obstar metallicity option works.

---

stars_optimize1.in

optimizer on stellar grids

```
title optimizer on stellar grids
#
# commands controlling continuum =========
table star tlusty ostar 3-dim 31200 3.6 -1.12 vary
ionization par -3
#
# commands for density & abundances =========
hden 4 vary
init file "hheonly.ini"
element oxygen on
#
# commands controlling geometry =========
case B
stop zone 1
#
# other commands for details =========
optimize tolerance 0.03
constant temper 4.3 vary
optimize phymir sequential
optimize iteration 750
# the following spectrum was derived by running this sim at hden 5, t=4,
# and T_star=51200
# resulting eden was 5.040 and T=4, which we shall assert that we find
optimize lines
O 2 3728.81 0.0446
O 2 3726.03 0.1164
Blnd 7323 0.1237
Blnd 7332 0.1018
O 3 5006.84 10.0205
O 3 4363.21 0.0968
end of lines
#
# commands controlling output =========
print line faint -2
#
save overview "stars_optimize1.ovr"
```

```
save performance "stars_optimize1.per"
#
# optimize_phymir.in
# class optimizer
# ======================================
#
```

This checks whether the optimizer sets corrects limits for Teff. The line spectrum was calculated at T = 1e4 K, n_H=1e5 cm^-3, T_star = 51200 K.

---

stars_optimize2.in

optimizer on stellar grids

```
title optimizer on stellar grids
#
# commands controlling continuum =========
table star costar 36200 vary
ionization par -3
#
# commands for density & abundances =========
hden 4 vary
init file "hheonly.ini"
element oxygen on
#
# commands controlling geometry =========
Case B
stop zone 1
#
# other commands for details =========
optimize tolerance 0.03
constant temper 4.3 vary
optimize phymir sequential
optimize iteration 500
# the following spectrum was derived by running this sim at hden 5, t=4,
# and T_star=51200
# resulting eden was 5.041 and T=4, which we shall assert that we find
optimize lines
O 2 3728.81 0.0365
O 2 3726.03 0.0951
Blnd 7323 0.1012
Blnd 7332 0.0833
O 3 5006.84 10.4461
O 3 4363.21 0.1010
end of lines
#
# commands controlling output =========
print line faint -2
#
save overview "stars_optimize2.ovr"
save performance "stars_optimize2.per"
#
# optimize_phymir.in
# class optimizer
# ======================================
#
```

This checks whether the optimizer sets corrects limits for Teff. The line spectrum was calculated at T = 1e4 K, n_H=1e5 cm^-3, T_star = 51200 K.

---

stars_optimize3.in

optimizer on stellar grids

```
title optimizer on stellar grids
#
# commands controlling continuum =========
table star costar age 5.8 log 36 msol vary
ionization par -3
#
# commands for density & abundances =========
hden 4 vary
init file "hheonly.ini"
element oxygen on
#
# commands controlling geometry =========
Case B
stop zone 1
#
# other commands for details =========
optimize tolerance 0.03
constant temper 4.3 vary
optimize phymir sequential
optimize iteration 500
# the following spectrum was derived by running this sim at hden 5, t=4,
# and log(age)=6.3
# resulting eden was 5.040 and T=4, which we shall assert that we find
optimize lines
O 2 3728.81 0.0680
O 2 3726.03 0.1774
Blnd 7323 0.1887
Blnd 7332 0.1554
O 3 5006.84 8.7015
O 3 4363.21 0.0841
end of lines
#
# commands controlling output =========
print line faint -2
#
save overview "stars_optimize3.ovr"
save performance "stars_optimize3.per"
#
# optimize_phymir.in
# class optimizer
# ======================================
#
```

This checks whether the optimizer sets corrects limits for log(age). The line spectrum was calculated at T = 1e4 K, n_H=1e5 cm^-3, log(age/yr) = 6.3.

---

stars_ostar2002.in

tlusty O star grid

```
title tlusty O star grid
#
# commands controlling continuum =========
# Approximate model of a hot star ionizing its surroundings.
# Assume H density of 1e+6 per cc. This run tests the new Tlusty model option.
# I choose the T_eff and log(g) values arbitrarily. It implies a star
# with luminosity 32300 L_sun, radius 6.4745 R_sun, and mass 3.745 M_sun.
table star tlusty ostar 30400.0 4.2
luminosity 4.509202522 solar
#
# commands for density & abundances =========
```

```
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -3.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
no blends
#
# in this model the Lyman lines are pumped significantly by the stellar continuum;
# disable this process to avoid critical dependence on the precise shape of the continuum.
no induced processes
constant temperature 4
#
# commands controlling output =========
#
save performance "stars_ostar2002.per"
save overview last "stars_ostar2002.ovr"
save results last "stars_ostar2002.rlt"
save continuum last "stars_ostar2002.con" units angstrom
save transmitted continuum last "stars_ostar2002.trn" no header
#
# stars_ostar2002.in
# class stars
# ======================================
```

This is a test that the code can correctly access the large block of Tlusty O-star model atmosphere continua.

Checks: table star tlusty ostar command works.

---

stars_ostar2002_3d.in

tlusty Ostar grid

```
title tlusty Ostar grid
#
# commands controlling continuum =========
# Approximate model of a hot star ionizing its surroundings.
# Assume H density of 1e+6 per cc. This run tests the new Tlusty model option.
# I choose the T_eff, log(g) and log(Z) values arbitrarily.
table star tlusty ostar 3-dim 30400.0 4.2 -1.573
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -3.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
#
# in this model the Lyman lines are pumped significantly by the stellar continuum;
# disable this process to avoid critical dependence on the precise shape of the continuum.
no induced processes
constant temperature 4
```

```
no blends
#
# commands controlling output =========
#
save performance "stars_ostar2002_3d.per"
save overview last "stars_ostar2002_3d.ovr"
save results last "stars_ostar2002_3d.rlt"
save continuum last "stars_ostar2002_3d.con" units angstrom
save transmitted continuum last "stars_ostar2002_3d.trn" no header
#
# stars_ostar2002_3d.in
# class stars
# ======================================
```

This is a test that the code can correctly access the large block of Tlusty O-star model atmosphere continua.

Checks: table star tlusty ostar 3-dim command works.

---

stars_ostar2002_all.in

tlusty Ostar grid

```
title tlusty Ostar grid
#
# commands controlling continuum =========
# Approximate model of 10 hot stars ionizing their surroundings.
# Assume H density of 1e+6 per cc. This run tests all the various
# metallicities contained in the OSTAR 2002 grids. I choose the T_eff
# and log(g) values such that the selection algorithm gets a good workout.
table star tlusty ostar Z+0.3 30000.0 4.5
luminosity 4.509202522 solar
table star tlusty ostar Z+0.0 31400.0 4.5
luminosity 4.509202522 solar
table star tlusty ostar Z-0.3 45000.0 4.2
luminosity 4.509202522 solar
table star tlusty ostar Z-0.7 30400.0 4.2
luminosity 4.509202522 solar
table star tlusty ostar Z-1.0 27500.0 3.0
luminosity 4.509202522 solar
table star tlusty ostar Z-1.5 55000.0 4.75
luminosity 4.509202522 solar
table star tlusty ostar Z-1.7 27500.0 4.75
luminosity 4.509202522 solar
table star tlusty ostar Z-2.0 55000.0 3.00
luminosity 4.509202522 solar
table star tlusty ostar Z-3.0 44400.0 3.2
luminosity 4.509202522 solar
table star tlusty ostar Z-INF 53000.0 4.75
luminosity 4.509202522 solar
table star tlusty ostar Z+0.0 48400.0 3.87
luminosity 4.509202522 solar
table star tlusty ostar Z-0.7 48400.0 3.55
luminosity 4.509202522 solar
table star tlusty ostar Z+0.3 43400.0 3.65
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -2.0 parsec
sphere
```

```
stop zone 1
set dr 0
#
# other commands for details =========
#
# in this model the Lyman lines are pumped significantly by the stellar continuum;
# disable this process to avoid critical dependence on the precise shape of the continuum.
no induced processes
constant temperature 4
no blends
#
# commands controlling output =========
#
save performance "stars_ostar2002_all.per"
save overview last "stars_ostar2002_all.ovr"
save results last "stars_ostar2002_all.rlt"
save continuum last "stars_ostar2002_all.con" units angstrom
save transmitted continuum last "stars_ostar2002_all.trn" no header
#
# stars_ostar2002_all.in
# class stars
# ======================================
```

This is a test that the code can correctly access the large block of Tlusty O-star model atmosphere continua.

Checks: table star tlusty ostar metallicity option works, also test selection algorithm.

---

stars_rauch_3d.in

Rauch 3-dimensional grid

```
title Rauch 3-dimensional grid
#
# commands controlling continuum =========
table star rauch 3-dim T = 150000 K, g = 6.5 , log(Z) = -0.6
luminosity 4.5 solar
table star rauch old 3-dim T = 233000 K, g = 7.5 , log(Z) = -0.32
luminosity 4.5 solar
#
# commands controlling geometry =========
sphere
radius 18
stop zone 1
set dr 0
#
# commands for density & abundances =========
abundances planetary
hden 3.0
#
# other commands for details =========
no level2
no blends
#
# commands controlling output =========
save performance "stars_rauch_3d.per"
save overview last "stars_rauch_3d.ovr"
save results last "stars_rauch_3d.rlt"
save continuum last "stars_rauch_3d.con" units angstrom
#
# stars_rauch_3d.in
# class stars
# ======================================
```

This model checks that the code is able to access the 3-dim versions of the Rauch grids of stellar atmosphere models. Constant temperature is set since this test is intended to test shape of ionizing continuum, not thermal physics.

---

stars_rauch_cowd.in

Rauch hot PN star

```
title Rauch hot PN star
#
# commands controlling continuum =========
table star rauch co wd T = 238000 K
luminosity 4.5 solar
#
# commands controlling geometry =========
sphere
radius 18
stop zone 1
set dr 0
#
# commands for density & abundances =========
abundances planetary
hden 3.0
#
# other commands for details =========
no level2
no blends
# test adding continuum points
set nfnu add 10 cm
set nfnu add 350 micron
set nfnu add 200 angstrom
#
# commands controlling output =========
save performance "stars_rauch_cowd.per"
save overview last "stars_rauch_cowd.ovr"
save results last "stars_rauch_cowd.rlt"
save continuum last "stars_rauch_cowd.con" units angstrom
#
# stars_rauch_cowd.in
# class stars
# ======================================
```

This is a model of a very hot planetary nebula, and checks that the code is able to access the C/O white dwarf version of the Rauch grid of stellar atmosphere models.

---

stars_rauch_h+he.in

Rauch PN central star

```
title Rauch PN central star
#
# commands controlling continuum =========
# this tests the various interpolation modes of the 3d grid
table star rauch h+he T = 150000 K, g = 6.5 , f(He) = 0.2
luminosity 4.5 solar
table star rauch h+he T = 155000 K, g = 6.5 , f(He) = 0.2
luminosity 4.5 solar
table star rauch h+he T = 150000 K, g = 6.25 , f(He) = 0.2
luminosity 4.5 solar
table star rauch h+he T = 150000 K, g = 6.5 , f(He) = 0.25
luminosity 4.5 solar
table star rauch h+he T = 155000 K, g = 6.25 , f(He) = 0.2
```

```
luminosity 4.5 solar
table star rauch h+he T = 155000 K, g = 6.5 , f(He) = 0.25
luminosity 4.5 solar
table star rauch h+he T = 150000 K, g = 6.25 , f(He) = 0.25
luminosity 4.5 solar
table star rauch h+he T = 155000 K, g = 6.25 , f(He) = 0.25
luminosity 4.5 solar
#
# commands controlling geometry =========
sphere
radius 18
stop zone 1
set dr 0
#
# commands for density & abundances =========
abundances planetary
hden 3.0
#
# other commands for details =========
no level2
no blends
#
# commands controlling output =========
save performance "stars_rauch_h+he.per"
save overview last "stars_rauch_h+he.ovr"
save results last "stars_rauch_h+he.rlt"
save continuum last "stars_rauch_h+he.con" units angstrom
#
# stars_rauch_h+he.in
# class stars
# ======================================
```

This is a model of a very hot planetary nebula, and checks that the code is able to access the H+He version of the Rauch grid of stellar atmosphere models.

---

stars_rauch_h-ca.in

Rauch central star hot PN

```
title Rauch central star hot PN
# NB
# this uses the H-Ca rauch atmospheres
#
# commands controlling continuum =========
table star old rauch T = 250000 K, g = 7.5
luminosity 4.5 solar
#
# commands controlling geometry =========
sphere
radius 18
stop zone 1
set dr 0
#
# other commands for details =========
no level2
no blends
#
# commands for density & abundances =========
hden 3.0
abundances planetary
#
# commands controlling output =========
save performance "stars_rauch_h-ca.per"
save overview last "stars_rauch_h-ca.ovr"
save results last "stars_rauch_h-ca.rlt"
```

```
save continuum last "stars_rauch_h-ca.con" units angstrom
#
# stars_rauch_h-ca.in
# class stars
# ======================================
```

This is a model of a very hot planetary nebula, and checks that the code is able to access the H-Ca Rauch grid of stellar atmosphere models.

---

stars_rauch_h-ni.in

Rauch hot PN star

```
title Rauch hot PN star
#
# commands controlling continuum =========
table star rauch T = 150000 K, g = 6.5
luminosity 4.5 solar
#
# commands controlling geometry =========
sphere
radius 18
stop zone 1
set dr 0
#
# commands for density & abundances =========
abundances planetary
hden 3.0
#
# other commands for details =========
no level2
no blends
#
# commands controlling output =========
save performance "stars_rauch_h-ni.per"
save overview last "stars_rauch_h-ni.ovr"
save results last "stars_rauch_h-ni.rlt"
save continuum last "stars_rauch_h-ni.con" units angstrom
#
# stars_rauch_h-ni.in
# class stars
# ======================================
```

This is a model of a very hot planetary nebula, and checks that the code is able to access the H-Ni version of the Rauch grid of stellar atmosphere models. Constant temperature is set since this test is intended to test shape of ionizing continuum, not thermal physics.

---

stars_rauch_helium.in

Rauch hot PN star

```
title Rauch hot PN star
#
# commands controlling continuum =========
table star rauch helium T = 240000 K, g = 8.5
luminosity 4.5 solar
#
# commands controlling geometry =========
sphere
radius 18
```

```
stop zone 1
set dr 0
#
# commands for density & abundances =========
abundances planetary
hden 3.0
#
# other commands for details =========
no level2
no blends
# test adding continuum points
set nfnu add 10 cm
set nfnu add 350 micron
set nfnu add 200 angstrom
#
# commands controlling output =========
save performance "stars_rauch_helium.per"
save overview last "stars_rauch_helium.ovr"
save results last "stars_rauch_helium.rlt"
save continuum last "stars_rauch_helium.con" units angstrom
#
# stars_rauch_helium.in
# class stars
# ======================================
```

This is a model of a very hot planetary nebula, and checks that the code is able to access the pure helium version of the Rauch grid of stellar atmosphere models.

---

stars_rauch_hydr.in

Rauch hot PN star

```
title Rauch hot PN star
#
# commands controlling continuum =========
table star rauch hydr T = 240000 K, g = 8.5
luminosity 4.5 solar
#
# commands controlling geometry =========
sphere
radius 18
stop zone 1
set dr 0
#
# commands for density & abundances =========
abundances planetary
hden 3.0
#
# other commands for details =========
no level2
no blends
#
# commands controlling output =========
save performance "stars_rauch_hydr.per"
save overview last "stars_rauch_hydr.ovr"
save results last "stars_rauch_hydr.rlt"
save continuum last "stars_rauch_hydr.con" units angstrom
#
# stars_rauch_hydr.in
# class stars
# ======================================
```

This is a model of a very hot planetary nebula, and checks that the code is able to access the pure hydrogen version of the Rauch grid of stellar atmosphere models.

---

stars_rauch_pg1159.in

Rauch hot [WR] PN

```
title Rauch hot [WR] PN
#
# commands controlling continuum =========
table star rauch pg1159 T=150000K g=6.5
luminosity 4.5 solar
#
# commands controlling geometry =========
sphere
radius 18
stop zone 1
set dr 0
#
# commands for density & abundances =========
abundances planetary
hden 3.0
#
# other commands for details =========
no level2
no blends
#
# commands controlling output =========
save performance "stars_rauch_pg1159.per"
save overview last "stars_rauch_pg1159.ovr"
save results last "stars_rauch_pg1159.rlt"
save continuum last "stars_rauch_pg1159.con" units angstrom
#
# stars_rauch.in
# class stars
# ======================================
```

This is a model of a very hot planetary nebula, and checks that the code is able to access the PG1159 version of the Rauch grid of stellar atmosphere models.

---

stars_rauch_pg1159_ascii.in

Rauch cool [WR] PN

```
title Rauch cool [WR] PN
#
# commands controlling continuum =========
table star "rauch_pg1159.ascii" T=40000K g=7
luminosity 4.5 solar
#
# commands controlling geometry =========
sphere
radius 18
stop zone 1
set dr 0
#
# commands for density & abundances =========
abundances planetary
hden 3.0
#
# other commands for details =========
no level2
set nfnu add 9.5 angstrom
no blends
#
```

```
# commands controlling output =========
save performance "stars_rauch_pg1159_ascii.per"
save overview last "stars_rauch_pg1159_ascii.ovr"
save results last "stars_rauch_pg1159_ascii.rlt"
save continuum last "stars_rauch_pg1159_ascii.con" units angstrom
#
# stars_rauch_pg1159_ascii.in
# class stars
# ======================================
```

This is a model of a cool PNCS, and checks that the code can correctly rebin a model with zero fluxes embedded. It also exercises reading directly from an ascii file.

---

stars_starburst99.in

Starburst 99 SED

```
title Starburst 99 SED
#
# commands controlling continuum =========
# read the table starburst and interploate to an age of 1e8 years
table star log age=8 "starburst99.mod"
luminosity 43
# add background continuum - starburs 99 does not extend
# into fir so code would complain about zero continuum
# adding the cosmic background stops this complaint
background
#
# commands for density & abundances =========
hden 5
#
# commands controlling geometry =========
stop zone 1
radius 20
#
# other commands for details =========
constant temper 4
no blends
#
# commands controlling output =========
save overview "stars_starburst99.ovr"
save performance "stars_starburst99.per"
save continuum last "stars_starburst99.con" units angstrom
#
#
# stars_starburst99.in
# class stars
# ======================================
#
```

this is a demonstration of the use of a Starburst 99 spectrum. It was provided to me by anand Srianand, and we used it in Srianand et al. 2003. A constant temperature is set since this is to test shape of continuum not thermal physics. It also tests access to user-supplied grids as the mechanism is the same.

---

stars_starburst99_2d.in

Starburst 99 2D SED

```
title Starburst 99 2D SED
#
```

```
# commands controlling continuum =========
# read the table starburst and interpolate to an age of 2.09e6 years
# and a metallicity of 12.
table star log age=6.32 Z=12. "starburst99_2d.mod"
luminosity 43
# add background continuum - starburs 99 does not extend
# into fir so code would complain about zero continuum
# adding the cosmic background stops this complaint
background
#
# commands for density & abundances =========
hden 5
#
# commands controlling geometry =========
stop zone 1
radius 20
#
# other commands for details =========
constant temper 4
no blends
#
# commands controlling output =========
save overview "stars_starburst99_2d.ovr"
save performance "stars_starburst99_2d.per"
save continuum last "stars_starburst99_2d.con" units angstrom
#
#
# stars_starburst99_2d.in
# class stars
# ======================================
#
```

this is a demonstration of the use of a manually crafted Starburst 99 2D grid, allowing for interpolation in both age and metallicity. It was provided by Christophe Morisset. A constant temperature is set since this is to test shape of continuum not thermal physics. It also tests access to user-supplied grids as the mechanism is the same.

---

stars_werner.in

Werner stars grid

```
title Werner stars grid
#
# commands controlling continuum =========
table star werner 190000 g=7.5
luminosity total 38
#
# commands for density & abundances =========
hden 4
abundances planetary no grains
grains agm no qheat single
#
# commands controlling geometry =========
radius 17
sphere
set dr 0
stop zone 1
#
# other commands for details =========
constant temperature 4.373
no blends
#
# commands controlling output =========
#
save performance "stars_werner.per"
save overview last "stars_werner.ovr"
```

```
save results last "stars_werner.rlt"
save continuum last "stars_werner.con" units angstrom
save transmitted continuum last "stars_werner.trn"
#
# stars_werner.in
# class stars
# ======================================
#
```

This checks that the code can access Kevin Volk39s Werner atmospheres.

Checks:
- table star Werner atmosphere works. constant temperature is set to that this tests shape of stellar continuum

---

stars_wmbasic.in

wmbasic stellar SED

```
title wmbasic stellar SED
#
# commands controlling continuum =========
# Approximate model of a hot star ionizing its surroundings.
# Assume H density of 1e+6 per cc. This run tests the WMBASIC model option.
# I choose the T_eff, log(g), and log(Z) values arbitrarily.
table star wmbasic 30000.0 4.0 -0.3
luminosity 4.509202522 solar
table star wmbasic 32000.0 4.0 0.0
luminosity 4.509202522 solar
table star wmbasic 40000.0 3.6 -0.3
luminosity 4.509202522 solar
table star wmbasic 35000.0 4.0 -0.15
luminosity 4.509202522 solar
table star wmbasic 57000.0 4.0 0.0
luminosity 4.509202522 solar
table star wmbasic 37000.0 3.4 -0.3
luminosity 4.509202522 solar
table star wmbasic 32000.0 4.0 -0.1
luminosity 4.509202522 solar
table star wmbasic 36000.0 3.5 -0.12
luminosity 4.509202522 solar
#
# commands for density & abundances =========
abundances old solar 84
hden 6.0
grains ism
#
# commands controlling geometry =========
radius -2.0 parsec
sphere
stop zone 1
set dr 0
#
# other commands for details =========
#
# in this model the Lyman lines are pumped significantly
# by the stellar continuum; disable this process to avoid critical
# dependence on the precise shape of the continuum.
no induced processes
constant temperature 4
no blends
#
# commands controlling output =========
#
save performance "stars_wmbasic.per"
```

```
save overview last "stars_wmbasic.ovr"
save results last "stars_wmbasic.rlt"
save transmitted continuum last "stars_wmbasic.trn" no header
save continuum last "stars_wmbasic.con" units angstrom
save continuum bins last "stars_wmbasic.bin" no header
#
# stars_wmbasic.in
# class stars
# ======================================
```

This is a test that the code can correctly access the WMBASIC O-star model atmosphere continua.

Checks: table star wmbasic command works.

---

thin.in

"Thin coronal model"

```
title "Thin coronal model"
coronal equilibrium 1e6K
hden 0
stop thickness 0
iterate
save performance "thin.per"
# thin.in
# ============================
```

This tests whether a layer with thickness much smaller than any relevant lengthscale is modelled in a single zone

---

time_cool_cd.in

constant density cooling cloud

```
title constant density cooling cloud
#
# commands controlling continuum =========
coronal 3.4e7 K init time
#
# commands for density & abundances =========
# want nT = 2e6 K cm-3
hden 5.88e-2 linear
#
# commands controlling geometry =========
set dr 0
set nend 1
stop zone 1
#
# other commands for details =========
# number of time steps
iterate 300
stop time when temperature falls below 1e4 K
cosmic rays background
#
# commands controlling output =========
print line faint 2 log
print line cumulative
print ages
set save prefix "time_cool_cd"
save time dependent ".tim" no hash
save dt ".dt" no hash
```

```
save overview ".ovr" no hash
save cooling ".col" no hash
save heating ".het" no hash
save continuum units Angstroms ".con"
save cumulative continuum units Angstroms last ".concum"
#
# commands giving the asserts =========
#
# time_cool_cd.in
# class dynamics
# ======================================
#
```

test time dependent cooling at constant density

---

time_cool_cd_eq.in

constant density equilibrium cooling cloud

```
title constant density equilibrium cooling cloud
#
# commands controlling continuum =========
coronal 3.4e7 K init time
#
# commands for density & abundances =========
# want nT = 2e6 K cm-3
hden 5.88e-2 linear
#
# commands controlling geometry =========
set dr 0
set nend 1
stop zone 1
#
# other commands for details =========
# number of time steps
iterate 300
stop time when temperature falls below 1e4 K
# this will do equilibrium cooling
set dynamics populations equilibrium
cosmic rays background
#
# commands controlling output =========
print line faint 2 log
print line cumulative
print ages
set save prefix "time_cool_cd_eq"
save time dependent ".tim" no hash
save overview ".ovr" no hash
save cooling ".col" no hash
save heating ".het" no hash
save continuum units Angstroms ".con"
save cumulative continuum units Angstroms last ".concum"
#
# commands giving the asserts =========
#
# time_cool_cd_eq.in
# class dynamics
# ======================================
#
```

test time dependent equilibrium cooling at constant density

---

time_cool_cd_flux.in

constant density cooling cloud

```
title constant density cooling cloud
#
# commands controlling continuum =========
coronal 3.4e7 K init time
#
# commands for density & abundances =========
# want nT = 2e6 K cm-3
hden 5.88e-2 linear
#
# commands controlling geometry =========
set dr 0
set nend 1
stop zone 1
#
# other commands for details =========
# number of time steps
iterate 300
stop time when temperature falls below 1e7 K
cosmic rays background
#
# commands controlling output =========
print line faint 2 log
print line cumulative
print ages
set cumulative flux
set save prefix "time_cool_cd_flux"
#
# commands giving the asserts =========
#
# time_cool_cd_flux.in
# class dynamics
# ======================================
#
```

Test time dependent cooling at constant density. In time_cool_cd.in, the line emission accumulation is done by default by mass. In this sim, the accumulation is done by flux (see 'set cumulative' above). This sim is meant simply to exercise the 'set cumulative flux' command, so a full run to low temperatures is deemed unnecessary.

---

time_cool_cd_noaccu.in

constant density cooling cloud

```
title constant density cooling cloud
#
# commands controlling continuum =========
coronal 3.4e7 K init time
#
# commands for density & abundances =========
# want nT = 2e6 K cm-3
hden 5.88e-2 linear
#
# commands controlling geometry =========
set dr 0
set nend 1
stop zone 1
#
# other commands for details =========
# number of time steps
iterate 300
stop time when temperature falls below 1e7 K
```

```
cosmic rays background
#
# commands controlling output =========
normalize to "O 8" 18.9689A
print line faint -3 log
print ages
set cumulative off
set save prefix "time_cool_cd_noaccu"
#
# commands giving the asserts =========
#
# time_cool_cd_flux.in
# class dynamics
# ======================================
#
```

Test time dependent cooling at constant density. In time_cool_cd.in, the line emission accumulation is done by default by mass. In this sim, no accumulation is performed (see 'set cumulative' above). The final line fluxes are those of the last iteration. This sim is meant simply to exercise the 'set cumulative off' command, so a full run to low temperatures is deemed unnecessary.
