CMFGEN

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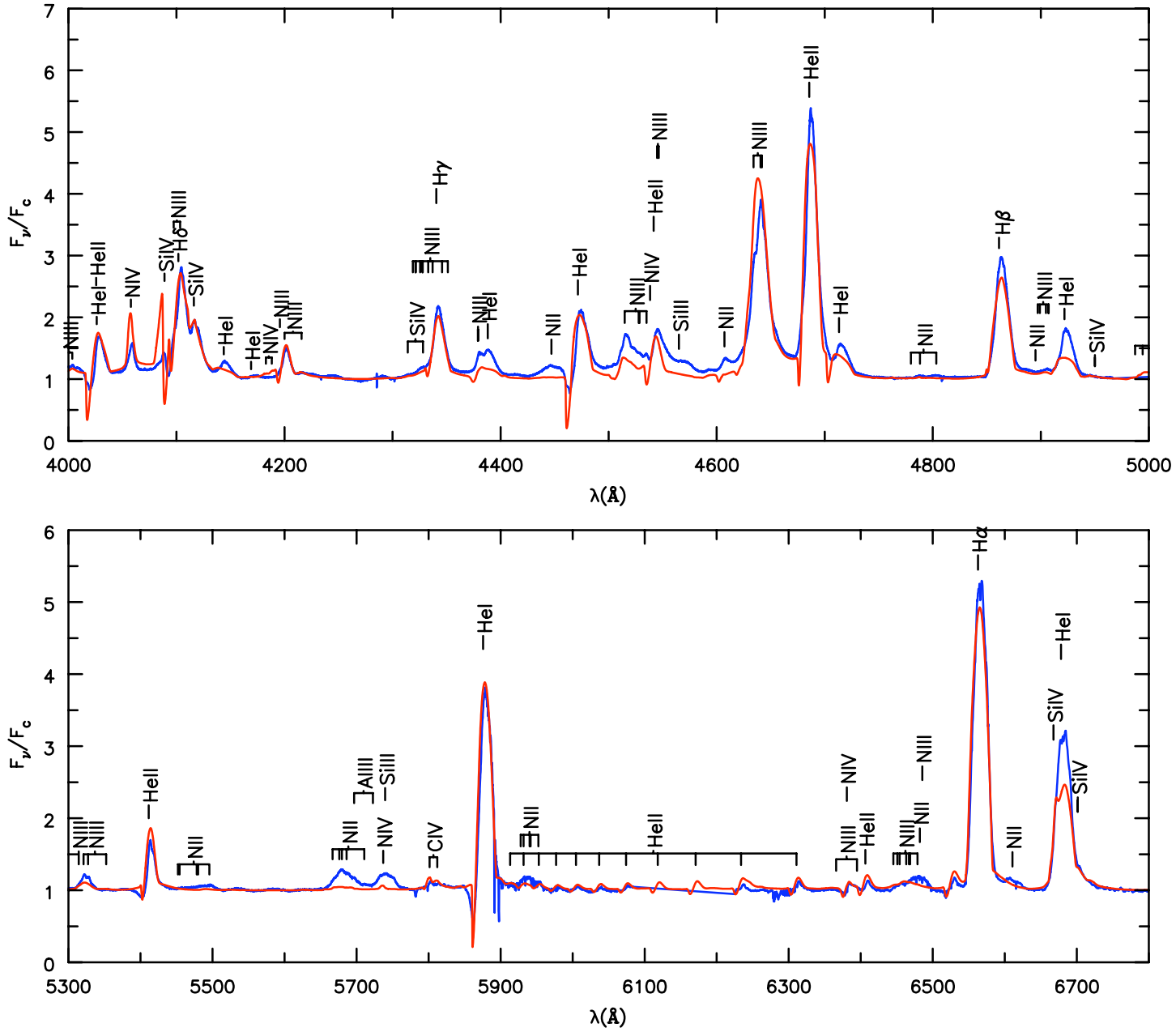
Name:

CoMoving Frame GENeral

Purposes

- Derive accurate stellar parameters and abundances for comparison with ``evolution'' calculations.
- Provide accurate EUV (i.e., $\lambda <$ 912 Å) radiation fields for input to nebular photoionization calculations.
- Provide fundamental data for the study of starbursts, star formation in galaxies, etc.
- Provide a better understanding of the hydrodynamics of winds.
- Provide distances to Type II SNe using the expanding photosphere method and its variants.
- Provide diagnostics of SNe which can place constraints on the progenitor and the explosion.
- Allow the development and testing of approximate methods that can be used in more complex geometries and in inhomogeneous media.

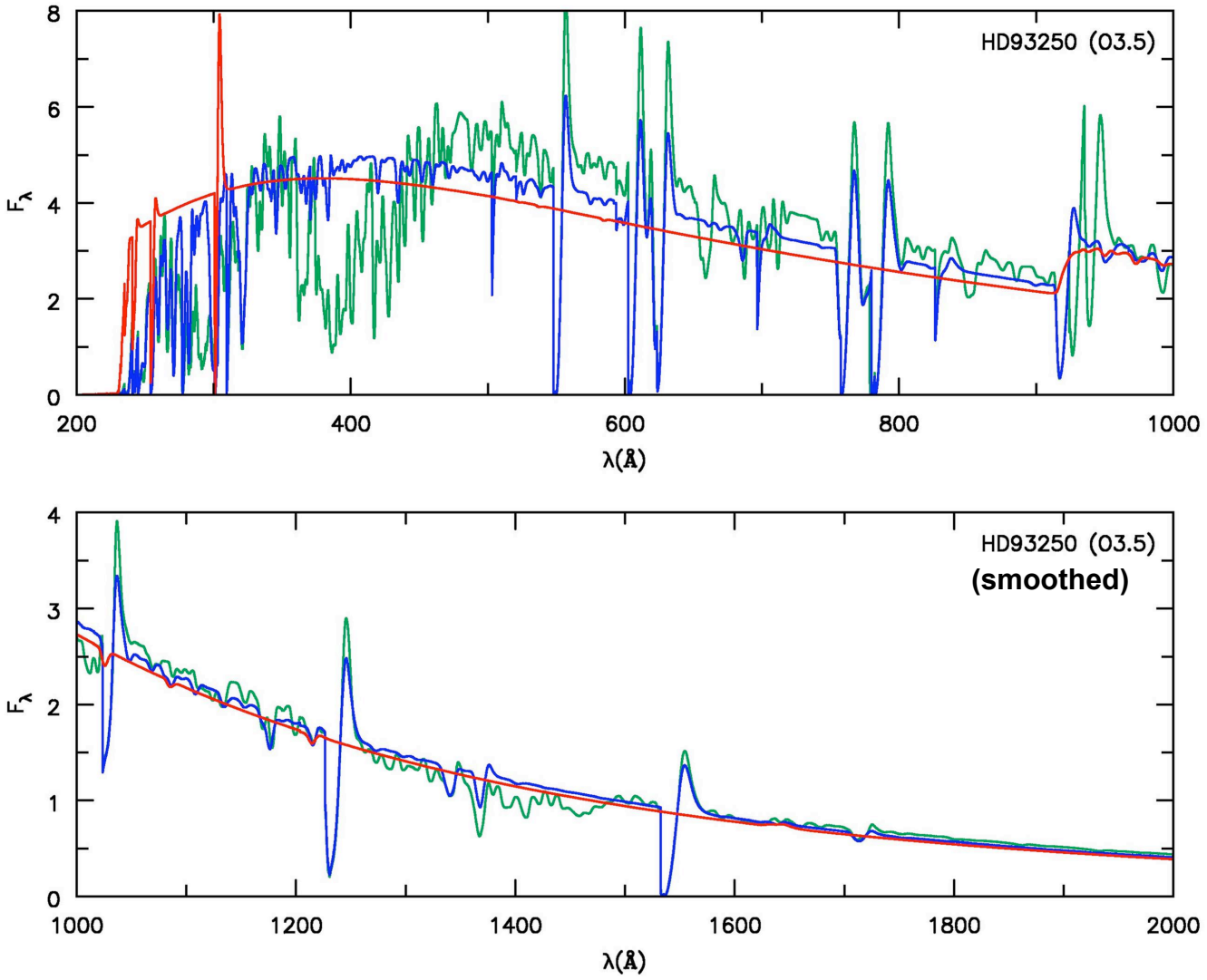


Herald, Hillier, and Schulte-Ladbeck, 2001

Effects of Line Blanketing on Energy Distribution

Key:

- H, He;
- H, He, CNO
- H, He, CNO, Fe, etc



HD93250

$L = 1.3 \times 10^6 L_\odot$, $T_{eff} = 45{,}700$ K, $R = 18.3 R_\odot$, log g = 4.0

$M = 5.6 \times 10^{-7} M_\odot$/yr , $V_\infty = 3000$ km s^{-1}

The Problem

1. Model atmosphere construction: ρ, T, N_i, N_e
    - Generally *insensitive* to atomic details:
        - gf values
        - intrinsic line profiles
        - coherent/incoherent scattering
    - Include all species
    - Include all lines, even those with bad gf values.

2. Precise spectroscopic analysis
    - Use fixed model atmosphere
    - Details matter
        - Individual lines constrain T_{eff}, log g, & abundances.
        - Accurate gf values (usually) essential.

Unfortunately, H, He, CNO, and Fe are strongly coupled to atmospheric structure.

Code Suite

CMFGEN	---	Wind structure, T, populations
CMF_FLUX	---	Spectral computation
DISPGEN	---	Display package for T, POPs, testing, etc
SPEC_PLT	---	Spectral comparisons
MAIN_LTE	----	Compute Roseland opacity for given composition, atomic model, atomic data.

After running CMGEN need to run CMF_FLUX in order to compute spectrum.
Done in (model)/obs directory.

Atomic Data

Opacity Project:

Seaton 1987; Hummer et al. 1993

Bob Kurucz

Bell and Kurucz (1995)

http://kurucz.harvard.edu

Keith Butler (Munich)

Sultana Nahar / Anil Pradhan

http://www.astronomy.ohio-state.edu/~nahar/nahar_radiativeatomicdata/index.html

NIST

http://www.nist.gov/pml/data/asd.cfm (Energy levels, f values, bib)

http://www.nist.gov/pml/pubs/atspec/index.cfm (Introduction to Atomic Spectroscopy)

CLOUDY (Ferland/Verner)

Charge exchange rates

Ground state photoionization cross-sections

+ many others

Atomic Data

Atomic data is stored in ASCII data files in unique directory:

/export/home/jdh/atomic/NIT/III/24mar07

niiicol.dat	collisional cross section
niiiosc_rev.dat	oscillator strengths / energy levels
niiiauto	autoionization rates
f_to_s_ls	Super-level designations
phot_sm_0_A.dat	Ground state photoionization cross-sections
phot_sm_0_B.dat	Excited state phot. cross-sect.

With the exception of H, later dates generally preferred.
Files are readable, and levels names related to spectroscopic designations.
New atomic data is generally stored under a new date.
(Unfortunately no uniform directory/file naming convention)

Data format is unique to CMFGEN. I have auxiliary routines which convert published atomic data into CMFGEN format. This is MESSY – published atomic data has different formats, different energy level names, and computed/names under different assumptions (LS coupling, intermediate coupling, jj coupling).

DO NOT ASSUME THE ATOMIC DATA FOR SOME-NON STANDARD SPECTRAL FEATURE IS CORRECT.

Transfer options

Plane-Parallel

- Formal and Moment equations

Plane-Parallel comoving-frame

- Monotonic vertical velocity field
- Radiation computed in frame moving with the gas
  - => Opacities and emissivities ``are'' isotropic.
- Formal and Moment equations
- Zero order in v/c (only retains v/c term that multiply $\delta/\delta\nu$ terms)

Spherical comoving-frame

- Radial monotonic velocity field
- Formal and Moment equations
- Zero order in v/c (only retains v/c term that multiply $\delta/\delta\nu$ terms)

Transfer options

Spherical comoving frame

- Fully relativistic but static monotonic flows (i.e., fast wind)
- Formal and Moment equations

Spherical time-dependent comoving-frame

- First order v/c
- Only valid for Hubble flow (v prop. to r as in SN explosion)
- Moment equation only.

$$\frac{1}{cr^3}\frac{D(r^3 J_\nu)}{Dt} + \frac{1}{r^2}\frac{\partial(r^2 H_\nu)}{\partial r} - \frac{\nu V}{rc}\frac{\partial J_\nu}{\partial \nu} = \eta_\nu - \chi_\nu J_\nu$$

$$\frac{1}{cr^3}\frac{D(r^3 H_\nu)}{Dt} + \frac{1}{r^2}\frac{\partial(r^2 K_\nu)}{\partial r} + \frac{K_\nu - J_\nu}{r} - \frac{\nu V}{rc}\frac{\partial H_\nu}{\partial \nu} = -\chi_\nu H_\nu$$

Spherical time-dependent, fully relativistic

- Monotonic velocity law
- Moment equation only (undergoing testing).

NB: $\frac{D}{Dt} = \frac{\partial}{\partial t} + v\frac{\partial}{\partial r}$

Linearization

The rate equations are non-linear. We solve this set of equations via linearization. Consider a non linear equation in 1 variable --- x. In general the equation can be written as:

$$f(x)=0$$

For some estimate x_1, $f(x_1)\neq 0$. We can compute a correction Δx using a Taylor expansion. To first order, we require

$$0 = f(x_1) + \Delta x\, f'(x_1) \quad (' \text{ denotes derivative}).$$

This gives

$$\Delta x = - f(x_1)/ f'(x_1) \qquad \text{(Newton-Raphson iteration)}$$

Thus:

$$x_2 = x_1 - (-\Delta x)$$

NB: The $-$ sign explains why the correction in the file STEQ_VALS are negative.

This can easily be extended to more than one variable. In this case:

$$\underline{\underline{B}} \,.\, \underline{\delta N} = -\underline{F}$$

In CMFGEN, B is called BA (ion components are SE(ID)%BA) and F is STEQ (ion components are SE(ID)%STEQ)

Constructing the BA matrix

In general a rate equation has the form

$f(N_1, N_2, N_3 \ldots N_{NT-2}, Ne, T, J_1, J_2, \ldots J_{NCF}, Z_{lu} \ldots) = 0$

In general the explicit dependence is local (except, e.g., if we have advection).

Linearize rate equations in terms of $\delta N_1, \delta N_2, \delta N_3 \ldots \delta N_{NT-2}$, δNe, δT, $\delta J_1, \delta J_2, \ldots \delta J_{NCF}$, δZ_{lu} etc. (NB: many of the terms will be zero ---there is little cross talk between species and photoionization rates go to zero below the ionization edge.)

We can eliminate the $\delta J_1, \delta J_2, \ldots \delta J_{NCF}$, δZ_{lu} using the linearized transfer equation (discussed earlier) and by linearizing the opacities and emissivities.

HOWEVER this elimination couples the linearized equations over depth (since the J, in principal, are determined by the populations at all depths).

(1) We can minimize the coupling by ignoring it (!).

At each depth we have a set of NT simultaneous equations. The solutions at each can be computed independently of other depths.

Constructing the BA matrix

(2) Alternatively we take into account the coupling with neighboring depths (TRIDIGONAL) approach). The gives a block-TRIDAGONAL set of simultaneous equation – each block matrix is NT.NT. Solved by matrix version of the THOMAS algorithm. In this approach we have ND.NT simultaneous equations to solve ---> ~60,000 coupled simultaneous equations.

NB: DIGAONAL: Higher stability when corrections are large.
TRIDIAGONAL: Converges faster.

The solution is carried out using LAPACK routines. But in both case we do 2 tricks:

(1) We adjust the elements of the BA matrix so that we solve for the fractional corrections (i.e., $\delta N/N$). ABSOLUTELY ESSENTIAL – it helps to prevent singular matrices.

(2) We apply LAPACK routines to precondition the simultaneous equations. Without (1) this does not work.

Since we are solving for $\delta N/N$, we don not need the correction to be of high precision. The corrections simply need to be reasonable so that we still get convergence (perhaps at the expense of more iterations).

Iteration cycle

CMFGEN has 5 type of iteration cycles --- each cycle provides new estimates of T , Ne, Ni, and the density (sometimes) density. In order of increasing computational effort:

1. NG Acceleration.

   Use previous iteration cycles to guess new estimates. When, how often, etc is uncertain.

2. Hydrostatic correction

   Adjusts density structure to better satisfy hydrostatic equilibrum.

3. BA matrix fixed.

   Done when corrections are small (<5%?), and sometime after full iterations.
   When corrections ``small'', equivalent to full linearization but MUCH faster.

4. Lambda Iteration

   Often done at start of iteration, and regularly when %changes are large.
   Stabilizes populations
   Linearize rate equations only – J held fixed when solving for the corrections.
   T is held fixed.

5. Full linearizaton

   Construct the BA matrix from first principals.

Crucial Input/Control Files

batch.sh

Runs job, assign atomic data files

MODEL_SPEC

ND

Atom specifications

VADAT

Input data and controls

IN_ITS

Controls iteration cycle – can edit while job is running.

XZV_IN

Starting estimates of departure coefficients for species XzV

RVSIG_COL

R, V, SIGMA (dV/dr-1) if doing hdyro model.

HYDRO_DEFAULTS

Controls hydrostatic iteration

Crucial Output Files

Populations

RVTJ (R, V, T, opacities, etc)

POPDUP (DUM=HYD, HE, CARB, etc)

These are used by DISPGEN, and CMF_FLUX

Scratch files

SCRTEMP (not ASCII)

POINT1 & POINT 2

These store results for each iteration. POINT# has a pointer which allows you to stop a model, and rewind it to an earlier iteration.

Spectrum

OBSFLUX

Observed spectrum (ν in 10^{15} Hz, F_ν in Jy for d=1 kpc)

Reasonable spectra for W-R stars --- not ideal for O stars.

No intrinsic line broadening – smearing due to numerical diffusion.

CHECKS

Convergence

OUTGEN : grep MAXIMUM OUTGEN (current largest change).
STEQ_VALS : Does RHS get smaller?
CORRECTION_SUM : Size distribution of corrections with depth

Radiative Equilibrium

STEQ_VALS : NT equation
OBSFLUX : Is L conserved?
GENCOOL : Is Electron E. B. satisfied?

Ionization equilibrium

XzVPRRR : Is ionization/recombination equilibrium satisfied

CMF_FLUX

Designed to compute spectrum for comparison with observation.

Done with high accuracy, and using accurate intrinsic line profiles.

Two steps (one program):

(1) Compute J in the CMF. Necessary to allow for the incoherent effects of electron scattering. This subroutine generates:

$J(r,\nu)$, $\eta(r,\nu)$, and $\chi(r,\nu)$

where v is the frequency in the CMF.

(2) Compute the spectrum in the observer's frame. Fully relativistic, but stationary. For the calculation, $J(r,\nu)$, $\eta(r,\nu)$, and $\chi(r,\nu)$ are mapped into the observer's frame --- mapping is angle dependent.

Extra grid points, rays, frequencies etc can be added to improve computational accuracy.

Control files: batobs.sh (uses ../batch.sh) and CMF_FLUX_PARAM_INIT.