RELEASE NOTES

Please run a few test models and report any difficulties.

Please report any compile difficulties. I cannot fix bugs/features if I don't know about them. The following summary of changes was hurriedly put together, and is incomplete. This list does not include trivial changes. Many subroutines were updated, and some additional subroutines were created. Some documentation has not yet been updated to reflect the changes. You can use $cmfdist/com/full_diff.sh to see all differences.

I very much appreciate those users who reported issues with the previous release.

A updated atomic data release will follow in the near future.

John Hillier

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30-Oct-2016

Major changes to CMFGEN.

Added H- (labelled HMI) as opacity source and ion.
Revision to handling of two-photon opacity. Can now be done exactly.
Improvements in parallelization.
Changes to time-dependent radiative transfer routines. More options for handling boundary conditions.
Improvement in differencing of DJ/Dt term — gives improved energy conservation for IIP models.
Bug fix for photoionization type 7 (not used much) in $cmfdist/newsubs/sub_phot_gen.f
New velocity law option (3) added to when revising hydrostatic structure.
X-ray flux for stellar models can be specified — filling factors are adjusted to match the requested X-ray luminosity.

New programs:

$cmfdist/misc/check_energy_cons.f
Allows any conservation to be checked in a sequence of time-dependent SN models.

$cmfdist/misc/extrtap_scr.f
Generates starting models for new SN model based on an time extrapolation of two previous models. Works well for type Ia models.

Improvements to the following auxiliary routines.

$cmfdist/misc/n_multi_merge.f
$cmfdist/misc/mod_cool.f
Estimate of calling time output.
$cmfdist/misc/plt_net.f (used to plot data from an XzVPRRR file).
$cmfdist/misc/plt_cmf_lum.f
$cmfdist/misc/plt_cool.f
$cmfdist/misc/rev_rdinr.f
$cmfdist/misc/rev_rvsig,.f
$cmfdist/new_main/mod_subs/adjust_r_grid_v4.f
$cmfdist/new_main/adjust_sn_r_grid.f
$cmfdist/new_main/subs/do_cmf_hydro_v2.f
$cmfdist/subs/rd_sn_data.f
$cmfdist/subs/two/two_phot_rate.f

Additional changes:

Additional options added to:
Plotting package
DISPGEN.

Bug fix for disp/plt_phot_sub.f

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30-Jun-2013

1. Hopefully fixed some convergence issues that arrow in the version released 22-Mar-2014.
The issues were compiler and machine dependent.

2 Some minor bug fixes --- do a difference with earlier vision to see changes.

3. On the MAC, there may be linking issues if using this years release (I have not checked the latest version). There is a bug with the linker -- some module files don't get found. Adding a statement like (use a unique variable name):

```
integer :: VPHOT_DATA_MOD = 1
```

to each of the affected modules apparently solves the problem. Routines that may need to be changed include:

```
new_subs/phot_data_mod.f
new_main/mod_subs/ang_qw_mod.f
new_main/mod_subs/chg_exch_mod_v3.f
new_main/mod_subs/control_variable_mod.f
new_main/mod_subs/line_vec_mod.f
new_main/mod_subs/nuc_iso_mod.f
new_main/mod_subs/opac_mod.f
stark/mod_subs/prof_mod.f
new_main/mod_subs/steq_data_mod
plane/mod_ray_mom_store.f
newsubs/xray_data_mod.f
```

4. With some intel compilers, there were some linking issues regarding programs in $cmfdist/spec_plt. The fix is to change the ordering of the libraries in the link (i.e., the creation of the executable), but its unclear why this is necessary.

22-Mar-2014

1. CMFGEN can now handle variable width Doppler profiles, and STARK profiles.This ability has to specifically requested by new VADAT options -- the default is to use fixed width Doppler profiles. For most situations, this is adequate, and is recommended. Because of this change, a new frequency grid is used.

2. Extra hidden parameters have been added to both VADAT and CMFGEN. These effect the computation primarily of Stark profiles: They are: V_PROF_LIM (indicates one sided extent of profile -- default is 5000 km/s for cmf_flux_v5.f and 3000 km/s for CMFGEN), MAX_PROF_ED (indicates the maximum electron density used in Stark profile computations - def=10^16 -- maximum of some tabulated data is 10^17.) & NORM_PROFILE which means that the stark profiles are normalized to have unit area before they are used -- essential for CMFGEN. See documentation for known issues.

3. A file WARNINGS has been introduced. This contains many of the routine diagnostic message and warnings that typically come with a CMFGEN calculation. As consequence OUTGEN is a lot cleaner.

4. Convergence of plane-parallel models with VINF has been fixed (issues arose when using NEW_VST_METH=T). Setting this FALSE for stars will give equivalent convergence to older versions, probably requires less memory, and may be preferred.

5. A program (set_new_sn_mod) is available to update the VADAT file from time step 1 to time step 2 (when many radiative transfer options must be changed). It can also be used to update the time and sequence number when moving to model time-step 3, etc.

6. Memory for line profiles in cmf_flux_v5.f and cmfgen.f is now dynamically allocated.

7. New options have been introduced to help convergence of SN models on the first time step. There also have been significant improvements to rev_rdinr.exe so that improve r-grids can be created (with spacing determined by both the step size in log(tau) and R.

8. Errors related to level names for collisional data are now ONLY output to CMFGEN when there is no matching name in the oscillator file.

9. Some collisional files have been updated -- mainly corrections to levels names. New files were not created, so save original atomic model directory structure if you want to repeat a calculation exactly. Not much effect on most stellar models.

10. The capabilities of the DO_NG_V2 routine have been expanded.

11. You can now specify the iteration cycle using the control file SPECIFY_IT_CYCLE. See documentation. No effect if file is not present.

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01-Jul-2013

This is a slightly extended release of the 25-Noc-2012 which never made it to my web site. Thus users should read the 25-Nov-2012 release notes. Most of the changes are relatively minor -- new options, parallelization updates, and a few code changes to facilitate compilations.

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25-Nov-2012

(1) LTE populations are now also installed in LOG format in CMFGEN and DISPGEN. This is a MAJOR change and required a change in many routines. Since some subroutines had different passed arguments, file version names were updated. This was done to facilitate SN models with large changes in temperature that have high ionization in the inner region, but much lower temperature and ionization in the outer regions.

(2) Atomic data files now contain links to the atomic data. This can be obtained from the MODEL file by doing grep "\[Reference\]" MODEL

(3) Routines for non-thermal ionization in SN are now included in the distribution.

(4) There were some issues with incorrect names in atomic data files. An error is now output to OUTGEN when this occurs (the atomic data files have been fixed). Unfortunately this error will also occur when using small atoms in which the appropriate levels has not been included.

(5) Penning ionization has been included. Only relevant to SN. Set [INC_PEN]=F in VADAT file.

(6) Some programs now write messages to the terminal in color.

(7) More options included in MAINGEN. Mainly for SN work. Documentation not yet updated. New options can be found by differencing $cmfdist/disp/maingen.f with older version.

(8) MOD_PRRR was updated and is now more sophisticated. This allows a more compact form
of the PRRR files to be output, and plotting.

(9) The normalized check for the FLUX (output at the end of OBSFLUX) is now obtained by integrating inwards (rather than outwards). Mainly relevant to SN models.

(10) More options added to VADAT file. These are read in by $cmfdist/new_main/mod_subs/rd_control_variables.f. Most of these are related to non thermal ionizations.

(11) A new key word ([NEW_VST_METH]) has been added to VADAT. At present its defaults is TRUE. This potentially could slow the code, and might cause convergence difficulties (its been tested but I can't test all regimes). It helps the convergence of Ia models. The current default is TRUE -- to get the current (i.e., old) behavior, set to FALSE.

(12) Program no longer write NETRATE, TOTRATE, and LINEHEAT on last iteration. To get these set [WRITE_RATES]=T in VADAT.

(13) A bug related to CHG exchange reactions was fixed. See $cmfdist/new_main/subs/chg/set_chg_lev_id_v4.f

(14) A bug was fixed relating to ADJUST_LINE_FREQ ins CMF_FLUX calculations.

(15) Modifications to $cmfdist/plane/jgrey_hub_ddt_v3.f. Modified to converge better and fixed bug (only important if did not converge).

(16) Additional plotting options added to $cmfdist/spec_plt/plt_scr.f. This routine allows, for example, variables to be plotted for different iterations of a currently running model.

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7_Apr-2011

Several important bug fixes, and improvements.

(1) A bug with RD_STORE_LOG was fixed. This could potentially read in a bad data value depending on the structure of the VADAT file. If [] were aligned, there was no problem.

(2) A bug with the X_ray cross-sections was found. L shell cross-sections were not being included for Si IV, PV and similar species (arose because for these species only 1 electron is ejected from the inner shell. Code was also updated to include M shell (p and s states) for Iron. Limited tests did not find huge changes.

A new file xray_phot_fits.dat replaces an older version in the $atomic/misc directory of the same name. It is the same data, but has an extra column. To read this file, with an older version of the code, you will need to change the length of STRING in $cmfdist/newsubs/xray_data_mod.f to 100 (or point to the older version of the file).

(3) The HYDRO_DEFAULTS file now has another keyword indicating how many iterations have been done -- change is transparent to user. An ERROR is ouput to OUTGEN on the final iteration if the hydrostatic structure is poor -- check HYDRO

In the HYDRO file make sure MAX_R is set. I also recommend that you use the OB_OPT to ensure a fine grid at the outer boundary. The crucial number is DTAU(2)/DTAU(1) -- the following sets the ratio to 25.

```
SPECIFY  [OB_OPT]
2  [NOB_PARS]
50.0D0[OB_P1]
2.0D0 [OB_P2]
100[MAX_R]
```

(4) It is now possible to put a file ADJUST_CORRECTIONS in the model directory.
If you put

```
    10:20 0.3 15  0.5
```

it will scale the corrections (full iterations only) at depths 10 through 20 by a factor of 0.3, and depth 15 by 0.5. This is -ve relaxation, and can facilitate convergence when level pops are oscillating. Particularly useful for O stars with low mass-loss rates. For O stars with low Mdots, and high Vinf, 80 or more depth points

are recommended.

(4) In $atomic there are three new X-ray files: gal_xray_hr.dat, smc_xray_hr.dat, lmc_xray_hr.dat. These were computed with the plasma emission code APEC for solar, and scaled solar abundances by Janos Zsargo. They should be use instead of the old rs data.

(5) CMFGEN and CMF_FLUX work successfully with PGF95 and OMP. Using 4 processes does improve computation time. Presently I am using /opt/pgi/osx86-64/10.8/bin/pgf95 on a MAC, and /usr/local/pgi105/linux86-64/10.5/bin/pgf95 on a LINUX system.

(6) On a 32-bit linux system I successfully compiled CMFGEN using GFROTRAN44 -- version 41 had issues.I did not try parallel processing.

(7) CMFGEN runs under INTEL but I have had issues (as yet unresolved) when OMP options were switched on. There is also may be the usual character issue in one or two routines -- explicitly specifying the string length solves these.

(8) $cmfdist/newsubs/subs/non_therm contains dummy routines only. This routines are still under development.

(9) When running ltebat.sh to compute the ROSSELAND mean opacity table, it is no longer necessary to change MODEL_SPEC. In fact, ltebat.sh could point to the files (MODEL_SPEC and VADAT) in the parent directory.

(10) A file CORRECTION_LINK has been added which can be used with CORRECTION_SUM. The file prints the largest corrections at 5 to 10 depths, and indicates the levels associated with these corrections.

(11) Improvements have been made to the cpmod command.`

(12) The INTEL compiler has an and off problem with some declarations. Seems to be version and operating dependent. If the newly compiled crashes quickly do the following:

Edit $cmfdist/newsubs/rdphot_gen_v2.f and replace
CHARACTER*(*) OSCDATE by CHARACTER(LEN=*) OSCDATE

Edit $cmfdist/newsubs/genosc_v8.f and replace
CHARACTER*(*) FILNAME by CHARACTER(LEN=20) FILNAME(N)

(13) A big with photoionization type 30/31 was fixed, but these aren't currently used

John

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17-June-2010

There have been many changes, especially with improvements of SN models. The SN stuff is still very much under development. Some of the changes, especially the non trivial, are listed below.

The frequency selection has changed slightly -- thus old EDDFACTOR files will not work with the new version of CMFGEN (unless using FIXED_J=T in VADAT/CMF_FLUX_PARAMA_INIT).

Additional OMP instructions have been added to many routines. Sometimes these cause problems related to compiler bugs (or features!). If issues, compile without OMP. CMFGEN will run a factor of 2 to 2.5 times
faster (pgf95 compiler) using 4 cpus. Additional CPUS don't increase the speed dramatically (yet). A much better gain is obtained with cmf_flux.

/unix/set_line_buffering.f added for use with PGF95 compiler. The subroutine forces unbuffered output (useful for OUTGEN). For intel compilers, you may need to create a dummy routine.

com/cpmod has been updated to copy a SN model so the same model can be rerun in a new directory.

Flourine, Scandium, Vanadium, and Barium have can now be treated (atomic data files not yet updated on web).

Addition options addedi to DISPGEN. See maingen.f -- Documentation still to be updated.

Additional options added to misc/do_ng_v2.f

LOWN option added to wr_f_to_s
Format of RVTJ has change. Should be transparent to CMFGEN users.

Significant changes to cmfgen_sub.f, mostly related to SN work. A large section of code was transferred to a subroutine (update_ba_for_line.f).

Updates to new_main/mod_subs/comp_j_blank.f. Mainly related to new SN calls.

Additional variables in new_main/mod_subs/rd_control_variables.f. Mainly related to SN studies.

new_main/subs/do_cmf_hydro_v2.f
  Updated: Now join velocity at 0.75 x (sound speed) - was 0.5
  TAU_REF can be a parameter in the file HYDRO_DEFAULTS (default is 2/3 - same as old version).

new_main/subs/solveba_v9.f replaces version new_main/subs/solveba_v8.f.
    Designed to better converge models in which a few levels at a few depths are limiting convergence. Tends to help, but still under development. A vector (10 values) showing increases and decreases is now output to CMFGEN.

Additional options added to cmf_flux (changes in rd_cmf_flux_controls.f)
 24-June-2009

Minor bug fix in subs/det_main_cont_freq.f. Will cause slight (but insignificant) changes of models.

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This release fixes a couple of bugs to the 26-May-2009 release. There have also been some additional changes. The most notable fixes to the 26-May-2009 versions were:

 (1) Correction to lte_hydro/det_r_grid_v2.f which fixed a grid issue that caused Tau(RMAX) to be less than requested value.

 (2) Correction to misc/rewrite_scr.f which fixed an issue when NITSF and IREC were unequal in POINT1 files.

Additional notes:

 (1) Be careful that FG and FD in the cur_cmf/Makefile_definitions are correctly defined. I also added F90nomp which solves a bug/feature with the PGF95 compiled on a Mac Pro. It general, it can be defined the same as F90.

 (2) In the web directory there is a file called CMFGENGuide.txt which was written in conjunction with Phil Massey and Kathryn Neugent. You might find this useful with O star modeling.

 (3) A collection of O star models has been placed on my WEB page. These are models of intermediate complexity, and can be used as basis for new models. The models are based on those of Fabrice Martins, although some parameters have been rounded, and the atomic models and atoms updated.

Please check the web site in a few weeks in case others notice some additional updates.

 26-May-2009

Note: Some transitions have inaccurate wavelengths. This can be due to the adopted atomic models, or inaccurate data. When computing observed spectra, you can place the correct wavelengths in a file and soft-link it to REVISED_LAMBDAS. An example file is in misc/REVISED_LAMBDAS_9apr08, which show the correct format for the file. The case shown is for Si IV, and arises because I have not split the 6z state into 6g and 6h.

(1) Significant changes and fixes to SN routines.

(2) Modified computation of the Eddington factor, f, for most routines. Mainly done to facilitate changes
to SN routines. Revised routines include MOM_JREL_V5 (instead of V3); MOM_J_CMF_V8 (instead of V6), FG_J_CMF_V11 (instead of v10)

(3) Improvements to det_r_grid_v2.f used by DO_HYDRO option. Extra grid points at outer boundary now inserted after new uniform grid has been created. Should lead to better grid definition.

(4) An alternative option has been installed to prevent SL's form causing problem when solving for the temperature distribution. Option is SCL_SL_OPAC in VADAT, and only one of SCL_SL_OPAC
and SCL_LN can be true. SCL_SL_OPAC scale emissivities/opacities used in CMFGEN to yield consistency (rather than just the cooling rates). Now give consistency with RHS of zero-moment
transfer equation. Primarily installed for SN.

(5) SL_OPTION, FL_OPTION, and IL_OPTION can be inserted into MODEL_SPEC. These options, if present, provide a method of splitting SL for ALL species, with editing the batch.sh file. Primarily installed
for SN models.

(6) A few routines have OMP instructions inserted. CMF_FLUX runs considerable faster with multiple process -- e.g., over a factor of 3 gain for 4 processors. Only the observer's frame calculation is faster for SN model that uses relativistic transfer.

(7) DC_INTERP_METHOD can now be set to RTX. In this case interpolation is done in Excitation Temperature space, rather than departurecoefficients.

(8) All comments in VADAT must now start with a !. Banks lines are still allowed. Strings with non-matching [ ] are flagged.

(9) Extrapolation of photoionization cross-sections to higher energy improved. Only affected a single ionization stage where a resonance occurred at the end of the tabulated cross-section.

(10) Parameters for CMF_FLUX now placed in a module --- CMF_FLUX_CNTRL_VAR_MOD rather than in CMF_FLUX_SUB.

(11) OBS_FRAME_SUB can now handle a hollow core. Done for late-time SN models only when DIF (i.e., Diffusion approximation) is set to zero.

(12) As always there are minor bug fixes, changes, cleaning etc. None should significantly affect modeling in most case. You can always use diff to find out what changes have been made to the code. If you execute com/full_diff.sh old_dist in the current distribution, you will get a difference listing of all Makefile, f files etc in Diff_sum

**** Check consistency routines ****

(1) A couple of routines have been inserted to check parameter consistency. This is becoming useful as more options installed.

(2) CMFGEN now outputs recommended value of T_MIN to OUTGEN. Setting T_MIN prevents floating underflow/overflow when including very ionization species such as CV.

(3) CMFGEN now outputs to OUTGEN an indication of whether additional ionization stages should be added (only for species included in model)

Additional routines: These routines are included in the release. In some cases they simply replace earlier versions. In other cases they create new functions.

disp: PAR_XOPAC.INC, set_dc_or_pop_or_tx.f, wr_crit.f

misc: ave_dc.f, plt_alpha.f

new_main/mod_subs:
check_param_consistency.f, comp_grey_v3.f, sub_sob_line_v3.f
check_ions_present.f, check_tmin.f, out_sn_pops_v3.f
set_rv_hydro_model_v2.f

obs:
check_cmf_flux_param_consis.f, cmf_flux_cntrl_var_mod.f
obs_frame_sub_v7.f, rd_cmf_flux_controls.f

plane:
characteristics_v2.f, cmf_formal_rel.f, cmf_formal_rel_v2.f
define_grid_v2.f, derivr.f, derivs.f, edd_jrel_var_v2.f
fg_j_cmf_v11.f, fine_chi_grid.f, fine_r_grid.f, get_moms_non_rel.f
get_moms_rel.f, h_weight.f, j_weight.f, jgrey_hub_ddt_v3.f
k_weight.f, mod_ray_mom_store.f, mod_space_grid_v2.f, mod_var_jrel_v2.f
mom_j_cmf_v8.f, mom_jrel_v5.f, n_weight.f, optdepth_v2.f
rel_variables.f, runge_kutta.f, solve_cmf_formal_v2.f, var_jrel_v2.f
var_mom_j_cmf_v9.f, var_mom_jext_cmf_v3.f, velocity_law.f

spec_plt:
plt_jh_cur.f

subs:
fdg_f_to_s_ns_v1.f, par_fun_v3.f, rd_f_to_s_ids_v2.f
regrid_t_ed_v2.f, regrid_tx_r.f, subs/write_vec.f

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30-Jun-2008

(1) Bug fix to $cmfdist/new_main/subs/adjust_pops.f (could cause a crash on some machines).

(2) Fixed a stack of write statements. A simple X cause troubles on some compilers. Also fixed a few other compiler sensitive statements.

(3) Altered CMFGEN so that a new species can be added almost automatically. Proceed as in documentation, but code will now automatically switch from USE_FIXED_J=T to USE_FIXED_J=F. Before doing the switch, the code will NOW automatically do a gray temperature correction unless the hidden variable, DO_GT_AUTO, is set to false in IN_ITS. Make sure GREY_SCL_FAC_IN is valid.

(4) Some other cleaning. You can always use diff to find out what changes have been made to the code.

(5) If you alter any module files, and have trouble running the code, do a clean, and recompile the code. Its possible I may have missed the dependencies of some routines on some modules.

27-May-2008

(1) As always there are minor bug fixes, changes etc. None should significantly affect modeling.

(2) Further improvements to Gauss-fitting option in PLT_SPEC. Designed to measure EWs in normalized multiple model spectra in a semi-automatic and automatic fashion.

(3) Options installed to allow hydrostatic structure to be updated automatically in CMFGEN. Seems to work fine provided not to close to L(edd).

(4) Users wishing to use the relativistic and time-dependent SN routines should contact me and/or Luc Dessart. These are still under development

and testing.

4-Feb-2008

(1) As always there are minor bug fixes, changes etc. None should significantly affect modeling.

(2) Improvements to plane-parallel routines.

(3) DO_AUTO_LAMBDA placed in IN_ITS. Does not have to be present -- default is TRUE. Allows CMFGEN to automatically switch from LAMBDA iterations, FIXED_J_.TRUE. etc automatically after sufficient convergence has been obtained. Starting a model with DO_LAMBDA=T (and DO_AUTO_LAMBDA=T) is now a preferred option.

(4) Improved convergence when there are extremely large corrections using LAMBDA iterations (e.g., when including X-rays).

(5) Significant changes to allow SN models to be computed including
   (a) Time variations of statistical equilibrium equations,
   (b) Inclusion of relativistic terms in transfer equation (moment equations only)
   (c) Time dependent radiative transfer.

These procedures are still under development and refinement, and still need rigorous testing (especially the last 2).

(6) Improvements to WIND_HYD to facilitate construction of RVSIG_COL files assuming a hydrostatic structure. Next version will have the hydrostructure option included in CMFGEN.

(7) Improved Gauss-fitting option in PLT_SPEC. Designed to measure EWs in normalized multiple model spectra in a semi-automatic fashion.

(8) Help files for DISPGEN, PLT_SPEC, WR_F_TO_S etc are now now accessible by a web page in $cmfdist/web.

Please report any problems or errors.