CHIANTI

An Astrophysical Database for Emission Line Spectroscopy

CHIANTI TECHNICAL REPORT No. 22

CHIANTI software for interfacing with emission measure codes

Version 0.5, 17-Jun-2021, Peter Young
Version 0.4, 16-Dec-2019, Peter Young
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1 Overview

Codes that derive the differential emission measure (DEM) or emission measure (EM) for astrophysical plasmas will take as input a set of emission line intensities or fluxes, and the set of theoretial contribution functions for those lines. This Technical Report describes some CHIANTI software to help standardize this process.

The basic steps are:

1. Measure the emission line parameters and store them in a text file.
2. Create a line identification file that is used to match CHIANTI line IDs with the emission line parameter file.
3. Compute level population lookup tables for all of the lines of interest [`ch_dem_write_lookup_tables`].
4. Compute contribution functions from the lookup tables for the lines of interest [`ch_dem_gofnt`].
5. Derive the DEM, and optionally optimize the element abundances.

The individual steps are described in the sections below, and Sects. 7.1–7.3 describe routines for specific types of DEM.

Note that the computation of population lookup tables is a critical part of the process, and this is described in more detail in CHIANTI Technical Report No. 16.

2 The DEM function

The DEM function, ϕ, is related to an emission line intensity, I, by

$$I = 0.1151\,\epsilon \sum_{k=1}^{k=n} G_k \phi_k T_k \tag{1}$$

where ϵ is the element abundance, G is the line's contribution function (derived with the CHIANTI routine `gofnt`), and T is the temperature. The expression assumes that the temperatures are spaced on intervals of 0.05 dex in log T. See CHIANTI Technical Report No. 3 for more details.

Generally we want to vary the ϕ_k to give the best fit to the set of line intensities. Since there are usually more temperature points than emission lines, a functional form for ϕ is often assumed. A simple case is a Gaussian DEM function (Sect. 7.1).

3 Element abundances

Element abundance ratios can be derived as part of the DEM minimization procedure, which can be useful for studying the FIP effect, for example. The routines need an initial set of abundances and these are taken from the file specified by the CHIANTI system variable `!abund_file`. You can over-ride this by directly specifying a CHIANTI format file with the `abund_file` keyword.

Table 1: Element abundance types used by the ch_dem software.

Type	Description
0	Used for elements with only one line. The abundance is determined algebraically from the DEM.
1	Used for the reference element. By default the element with the most lines. Can be specified with `ab_elt_fixed`.
2	The element abundance is free to vary in the minimization process.
3	A fixed abundance obtained from the abundance file. Only used if `/fixed_abund` is set.

If all of the emission lines belong to the same element, then the absolute abundance of this element is not constrained and so it will be set to the initial abundance value. If lines are available from two or more elements, however, it is possible to obtain relative abundances of the elements.

Consider the case where we have lines belonging to the iron ions Fe X–XIV, and a single line belonging to Si X. In this case, the minimization procedure essentially yields a DEM only from the iron lines, and the Si/Fe relative abundance is determined algebraically from Eq. 1.

In the case where there are lines from Si IX and Si X, however, then the silicon lines enter the minimization procedure such that the Si/Fe ratio is varied to find the best fit to both of the silicon lines.

To keep all of the elements' abundances fixed, there is the keyword `/fixed_abund`. To customize which elements have fixed abundances and which have variable abundances, there is the keyword `swtch_ab`. Appendix E gives more details.

In the `ch_dem` output, elements get assigned an abundance type between 0 and 3. Table 1 explains what these are.

4 Population lookup tables

In order to speed up the computation process for DEMs, the ch_dem software makes use of population lookup tables. These are described in CHIANTI Technical Report No. 16. If you use the *Solarsoft* IDL library then a set of lookup tables are available there and you do not have to do anything, unless you are accessing a density regime outside of that in the *Solarsoft* tables. (The software automatically checks if this is the case.)

If you are not using *Solarsoft*, then you can download the *Solarsoft* tables from:

http://chiantidatabase.org/chianti_download.html

You will then need to set the environment variable $CHIANTI_LOOKUP to point to the directory containing the tables.

You can generate your own set of tables, but this takes a long time (at least 24 hours)—see CHIANTI Technical Report No. 16.

A quicker method is to generate your own tables only for the ions and transitions that you are interested in. To do this, define an environment variable $CH_DEM_LOOKUP to point to a directory where you want to store the tables. The tables are written with the routine `ch_dem_write_lookup_tables`, which is described in Step 3 of Sect. 5. The advantages are that the lookup tables take up much less disk space, they are more quickly calculated, and they are read and processed more quickly than the full tables. Note that if you choose to add new ions or lines later, then `ch_dem_write_lookup_tables` automatically updates the tables or adds new ones.

5 Preparation

Step 0. Read Sect. 4 and make sure you have population lookup tables. If you decide to create your own lookup tables, then Step 3 below will create them for you, although you will have to set the $CH_DEM_LOOKUP variable (see Sect. 4).

Step 1. The user first creates two text files: one contains the list of lines and their CHIANTI identifications (we call this `line_list.txt`), and the second contains a list of measured wavelengths, intensities and intensity errors (we call this `line_fits.txt`). The formats of these files are described in Appendices B and C.

Step 2. Now read the two text files, storing the information in an IDL structure:

```
line_data=ch_dem_read_line_ids('line_list.txt',int_file='line_fits.txt')
```

Step 3. Process the lookup tables:

```
ch_dem_write_lookup_tables,line_data,/execute
```

If you already have lookup tables (e.g., from *Solarsoft*) then this routine does not create new ones, instead it will check each ion to make sure the lookup table is available. The routine does create the file `pop_lookup_line_list.txt` in the current working directory, which is needed for the DEM routines (so do not skip this step!).

6 Line blending scenarios

Line blending is when a "line" being used in the DEM analysis consists of two or more atomic transitions. There are three scenarios of interest:

1. The transitions belong to the same ion and are blended in the observed spectrum (i.e., they are measured as a single feature).
2. The transitions belong to the same ion but are separate spectral features.
3. The transitions belong to different ions and are blended in the observed spectrum.

Scenarios 1 and 2 are easily dealt with in the `line_list.txt`—see the examples for Fe XII (scenario 1) and Si X (scenario 2) in Appendix B.

Scenario 3 is not handled by the `ch_dem` software. It is recommended that the user separates the blends prior to performing the DEM analysis. For example, suppose a spectral feature consists of a Fe X transition and a Fe XIV transition. The spectrum may contain an additional, unblended Fe XIV transition that can be used to estimate the contribution of Fe XIV to the blend. The de-blended Fe X intensity can then be used in the DEM analysis.

7 The DEM codes

Currently there are three types of DEM that are implemented, each with its own IDL routine. These are described in the subsections below.

One common feature of the examples is the use of the `interr_scale` optional input. Quite often with solar data the uncertainties resulting from fitting the emission lines can be very small because of high signal-to-noise. < 1 % is not untypical. Using these uncertainties in the DEM analysis can cause problems as the DEM solution is highly unlikely to fit the intensity data to within 1σ of the intensities. This can cause unusual DEM results to be returned.

The line fitting uncertainties are only one component of the overall uncertainties. For example, there will be uncertainties with the spectrometer's radiometric calibration and uncertainties with the atomic data. A crude way of capturing these additional uncertainties is to assign a blanket percentage uncertainty to each line. 15–20% is typical. With the `ch_dem` software this is done by specifying `interr_scale`. A value of 0.15 corresponds to 15%.

A common routine for plotting the output DEM and over-plotting the emission lines is `ch_dem_plot`, which is called as:

```
p=ch_dem_plot(output)
```

and produces an IDL plot object.

7.1 Gaussian DEMs

A routine called `ch_dem_gauss_fit` is available for fitting a Gaussian-shaped DEM to the line intensities. The form of the DEM is:

$$\phi_i = \frac{\mathrm{EM}_0}{\sigma_T\sqrt{2\pi}} \exp\left[-\frac{(T_i - T_0)^2}{2\sigma_T^2}\right] \tag{2}$$

which comes from Warren & Brooks (2009).

Following the preparation described in Sect. 5, an example call to the routine is:

```
output=ch_dem_gauss_fit(line_data,ldens=8.5,interr_scale=0.15)
```

7.2 Multi-linear DEMs

Another simplified treatment of DEMs is to assume a linear (or multi-linear) form. That is, the DEM is assumed to consist of one or more segments that are linear in log T–log ϕ space. This was

the approach used by Young (2005a), Young (2005b) and Young (2018) for an analysis of Mg, Ne and O emission lines observed by SOHO/CDS.

The setup using `ch_dem_read_line_ids` and `ch_dem_write_lookup_tables` is the same, the DEM is derived with, e.g.,

```
output=ch_dem_linear_fit(line_data,ldens=8.5,interr_scale=0.15,
          ltemp_nodes=[5.0,5.6,6.1])
```

The input `ltemp_nodes` specifies the node points for the DEM segments in log T. In the example, there will be two linear segments: one from log $T = 5.0$ to 5.6, and the second from log $T = 5.6$ to 6.1. More or less segments can be specified by simply adding or removing points from the input array.

7.3 Markov-Chain Monte Carlo method (MCMC) DEMs

The MCMC method was described by Kashyap & Drake (1998) and has been widely used in both astrophysics and solar physics. Unlike the Gaussian and multi-linear methods described above, the DEM does not have a specific functional form. The DEM is derived by doing, e.g.,

```
output=ch_dem_mcmc(line_data,ldens=8.5,interr_scale=0.15)
```

For this to work, the user must have the PINTofALE software installed. *This package is not part of Solarsoft* and must be installed from the PINTofALE webpage. I recommend that users remove the PINTofAlE/pro/external directory as this causes problems for the CHIANTI routines.

WARNING: the PINTofALE package has some routine clashes with Solarsoft and it is not recommended that you permanently attach the PINTofALE software to your IDL path. Instead, start a specific IDL session with the PINTofALE package at the front of your IDL path, and only use this for PINTofALE work.

The MCMC process may take some time to derive a DEM and information is printed to the screen and displayed in plots.

The `ch_dem_mcmc` routine automatically works out the temperature range of the DEM from the temperatures of formation of the emission lines.

8 Example and DEM comparison

A data-set from Hinode EIS was used to compare the results from the three DEM methods described in Sect. 7. The line intensities are given in Appendix G, and they were measured from a coronal hole observation of Hinode/EIS 2007 July 29 beginning at 23:21 UT.

The `line_data` structure was created as described in Sect. 5, and it was then input to the three `ch_dem` routines described in Sect. 7. For each, `int_err_scale` was set to 0.15 and a constant pressure of $\log(N_{\rm e}T) = 14.95$ (units: K cm^{-3}) was used (taken by deriving a density using the Fe XII λ186.9/λ195.1 ratio).

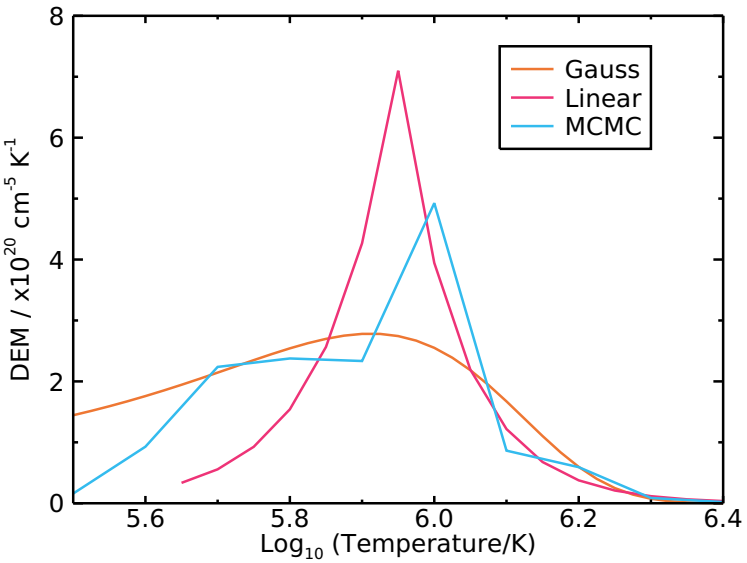

Figure 1: The DEMs returned by the routines ch_dem_gauss_fit (Gauss), ch_dem_linear_fit (Linear) and ch_dem_mcmc (MCMC).

The resulting DEMs are plotted in Figure 1. The highly-peaked DEM from the linear method arises because the DEM is defined in log T–log ϕ space and the plot shows log T vs. ϕ. The MCMC DEM shows a more complex shape, consistent with the lack of a pre-defined functional form.

Despite the differences in the DEM curves, a comparison of the model intensities with the observed values (Table 2) shows very good agreement. Note that, since there is only one line each from sulfur and silicon, then their abundances are adjusted to force them to fit on the DEM derived from the iron ions. The resulting abundance ratios from the three methods are shown in Table 3, which again show good agreement between the methods. Also shown are the solar photospheric and coronal abundance ratios from "scott_2015" and "schmelz_2012" abundance files in CHIANTI. These suggest that Si is under-abundant compared to Fe, and S has a coronal abundance.

Note that the intensity and abundance data are stored in the "line_data" and "abstr" tags of the output structure from the DEM routines.

References

Kashyap, V., & Drake, J. J. 1998, ApJ, 503, 450

Warren, H. P., & Brooks, D. H. 2009, ApJ, 700, 762

Young, P. R. 2005a, A&A, 439, 361

—. 2005b, A&A, 444, L45

—. 2018, ApJ, 855, 15

Table 2: Comparison of observed intensities with those derived from the three DEM codes.

		Intensity (erg cm^{-2} s^{-1} sr^{-1})			
Ion	Wavelength (Å)	Observed	Gauss	Linear	MCMC
si_10	258.37	3.6 ± 0.5	3.6	3.6	3.6
s_10	264.23	1.5 ± 0.3	1.5	1.5	1.5
fe_8	186.60	14.6 ± 0.5	16.3	13.9	15.8
fe_10	184.54	25.3 ± 0.9	14.7	19.7	18.1
fe_11	188.22	19.6 ± 0.7	22.8	23.2	23.1
fe_11	188.30	13.0 ± 0.7	13.8	14.0	14.0
fe_12	195.12	15.4 ± 0.3	19.3	15.5	16.6
fe_13	202.04	8.4 ± 0.4	6.4	5.0	5.8
fe_9	197.85	5.3 ± 0.2	3.6	5.0	4.3
fe_9	188.49	8.6 ± 0.3	8.0	10.9	9.5
fe_14	264.79	1.4 ± 0.2	1.4	1.2	1.4
fe_15	284.16	3.7 ± 0.7	3.6	4.9	4.5
fe_16	262.98	0.2 ± 0.2	0.0	0.1	0.1

Table 3: Abundances of silicon and sulfur relative to iron.

Method	Si/Fe	S/Fe
Gauss	0.51	0.23
Linear	0.55	0.25
MCMC	0.54	0.25
Photosphere	1.10	0.45
Coronal	1.02	0.24

A Document history

Version 0.5, 17-Jun-2021. Updated Sects. 3, 4 and 5, and Appendix E
Version 0.4, 16-Dec-2019. A number of updates following changes to the routines.
Version 0.3, 23-Jul-2019. Added Sect. 7.2.
Version 0.2, 18-Jul-2019. Added Sect. E.

B The line list file

This file contains a list of ion names, wavelengths and CHIANTI transitions. An example is:

```
si_7        275.36   1-6
si_10  a    258.37   2-10
si_10  a    261.06   2-9
fe_12       186.88   2-36,3-39
```

The Fortran format for the file is (a6,a2,f10.0,a40). The second column is optional and gives a string that tells the software that the lines should be summed together in the analysis. In the example above the two Si X lines will be summed and treated as a single line in the DEM analysis (this is scenario 2 discussed in Sect. 6). Any text symbols can be used in flagging the blends, and there is no restriction to how many lines can be blended.

The third column gives the wavelength of the line. This needs to be sufficiently precise that the software can match the line to observed lines in the line intensity file (App. C). Typically two decimal places is sufficient.

The fourth column gives the CHIANTI indices of the atomic transition corresponding to the emission line. To find the CHIANTI transition of the line you are interested in, use the routine `which_line`. For example,

```
  IDL> which_line,'si_7',275.36
       Wavelength   i   j  Lower level           Upper level             A-value
        272.647   1   7  2s2.2p4 3P2         - 2s.2p5 3P1             5.87e+09
        274.180   2   8  2s2.2p4 3P1         - 2s.2p5 3P0             1.38e+10
*       275.361   1   6  2s2.2p4 3P2         - 2s.2p5 3P2             1.02e+10
        275.675   2   7  2s2.2p4 3P1         - 2s.2p5 3P1             3.39e+09
        276.850   3   7  2s2.2p4 3P0         - 2s.2p5 3P1             4.46e+09
```

where it can be seen that the transition is 1–6. If a large list of lines appear when you run `which_line`, then use the keyword `/narrow` to use a reduced wavelength range for printing.

Blended lines of the same species require multiple transitions to be specified, separated by commas, as shown above for the 186.88 Å line of Fe XII. This is scenario 1 discussed in Sect. 6.

C The line intensity file

This file is specified to `ch_dem_read_line_ids` through the `int_file` optional input. The file is not required to be fixed format, but must contain three columns separated by white space. The first column is wavelength (angstroms), the second column is intensity, and the third column is the 1σ uncertainty on the intensity.

Note that the wavelengths are used to match the observed lines against those in the line list file (App. B). If the observed spectrum shows a systematic Doppler shift, then the lines may not correctly match. This can be fixed by specifying the input `vshift=` to `ch_dem_read_line_ids`. For example, if the observed spectrum has a Doppler shift of -50 km s^{-1} (blueshift) then `vshift=-50`. `ch_dem_read_line_ids` will print out the list of wavelength matches to the IDL screen so that velocity information can be checked.

If a particular line only has an upper limit, then this upper limit should be input as the intensity, and the error is set to -1. The software assumes that the intensity for the line is $I \pm I$, where I is the intensity. Note that upper limits are important for constraining the high temperature end of the DEM.

The `spec_gauss_widget` routine in *Solarsoft* allows 1D spectra to be manually fitted with Gaussians (there are "wrapper" routines for Hinode/EIS and IRIS called `spec_gauss_eis` and `spec_gauss_iris`).

The fits are stored in a text file with a standard format. In place of the three-column file described above, the user can use the `spec_gauss` output file by specifying the optional input `spec_gauss_int_file`:

```
IDL> line_data=ch_dem_read_line_ids('line_list.txt',
                  spec_gauss_int_file='spec_gauss_fits.txt')
```

D Storing radiative data

Using lookup tables for the level populations leads to large time savings compared to computing the contribution functions during the DEM calculation. An additional, smaller time-saving comes from storing the wavelength and A-values for the transitions in a data file, rather than reading them from the CHIANTI .wgfa file. For this reason, a file called `pop_lookup_line_list.txt` is written to the working directory containing the wavelengths and A-values. The routines `ch_dem_read_avals`, `ch_dem_write_avals` and `ch_dem_get_wvl_aval` do the job of reading, writing and processing these data. The `ch_dem` software handle this processing step automatically without need for input from the user.

E Element abundances in the minimization process

The behavior for handling element abundances in the minimization process varies depending on the number of different elements in the line list and the number of lines of each element, as mentioned in Sect. 3. The abundance information is processed with the routine `ch_dem_process_abund`, which takes the line list created by `ch_dem_read_line_ids` as input:

```
IDL> abstr=ch_dem_process_abund(line_data)
```

An information message will be printed to the IDL screen. The size of the output structure `abstr` corresponds to the number of elements. Each element is assigned a "type", i.e., a number between 0 and 3. See Table 1 for an explanation.

For the minimization process a 1D array of initial parameters is input to the MPFIT routines. The `ch_dem` routines will create an array containing the DEM parameters. For example, for a Gaussian function there are three parameters that define the Gaussian and each needs an initial guess. Thus the initial parameter array, `init`, contains three elements. By giving `init` as an input to `ch_dem_process_abund`, a new initial parameter (`out_init`) is returned with the abundance parameters to be varied appended. It is this initial parameter array that will be used in the minimization procedure. The example belows shows the calling procedure:

```
IDL> abstr=ch_dem_process_abund(line_data,init=init,out_init=out_init,
              abund_file=!abund_file)
```

Here the initial guesses for the abundances are taken from the default CHIANTI abundance file. This step is handled automatically by the `ch_dem` software, but is given here for information purposes.

In some cases you may want to specify exactly which elements to vary in the minimization procedure and which to keep constant. For example, you may decide to keep all of the low-FIP elements fixed and vary the high-FIP elements. For this there is the optional input `swtch_ab`. The best way to use this is to first run the `ch_dem` routines in the standard way, returning the output structure. One tag of the output structure is `abstr`. Consider the following:

```
IDL> print,output.abstr.elt_num,output.abstr.type
      14      16      26
       2       2       1
```

Here iron is the reference element (type 1) and the silicon and sulfur abundances are derived through the minimization procedure (type 2). We can force silicon to have a fixed abundance by doing:

```
IDL> swtch_ab=[0,1,0]
```

(Note that the reference element, iron, must be set to zero.) Now, giving `swtch_ab` as an input to the `ch_dem` routine, silicon will become a type 3 element (i.e., fixed abundance). Since the value 1 is specified for sulfur, then it continues to have a variable abundance.

F Notes on using the MCMC code

During the DEM optimization process, line intensities are computed from the DEM by the PINTofALE routine `lineflx.pro`. From a study of this routine, and comparing with Sect. 3.2 of CHIANTI Technical Report No. 3, I infer that the DEM is actually $\theta = \phi T N_{\rm e}/N_{\rm H}$ where ϕ is the DEM from Technical Report No. 3.

The hydrogen-to-electron ratio, $N_{\rm H}/N_{\rm e}$, can be computed as a function of temperature with the CHIANTI routine `proton_dens` and given as an optional input to the PINTofALE routine `mcmc_dem` with the keyword "nhne".

The contribution function is input to `mcmc_dem` through the "emis" input. This function is the same one as computed with the routine `ch_dem_add_contrib`.

G Example data-set

The line intensities from the 2007 July 29 Hinode/EIS data-set are given in Table 4. Note that the Fe XVI intensity is an upper limit.

Table 4: Measured line intensities from the Hinode/EIS 2007 July 29 data-set.

Ion	Wavelength (Å)	Intensity (erg cm^{-2} s^{-1} sr^{-1})
si_10	258.40	3.6 ± 0.5
s_10	264.27	1.5 ± 0.3
fe_8	186.63	14.6 ± 0.5
fe_10	184.56	25.3 ± 0.9
fe_11	188.25	19.6 ± 0.7
fe_11	188.33	13.0 ± 0.7
fe_12	195.15	15.4 ± 0.3
fe_13	202.08	8.4 ± 0.4
fe_9	197.89	5.3 ± 0.2
fe_9	188.52	8.6 ± 0.3
fe_14	264.81	1.4 ± 0.2
fe_15	284.20	3.7 ± 0.7
fe_16	263.01	0.2 ± 0.2