S(ME)^2: A Tutorial

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Abstract: SME (Spectroscopy Made Easy) [1] is a GUI-based tool for generating synthetic spectra of stars from atomic line lists and comparing them with observed spectra. It can be very useful in determining the abundances of elements in the solar atmosphere, as well as other parameters such as the surface gravity, gf values and micro- and macro-turbulence. Any one of these parameters may be chosen to vary by the user. SME then runs a Levenberg-Marquardt minimisation to determine the value of the parameter which produces a synthetic spectra that best matches the observed spectra. The proper calculation of the spectral lines is dependent upon having a correct set of atomic line data as input. Section 1 describes how to obtain this information. In Section 2, we generate a synthetic spectra using the line data requested with the all the original parameter values. Then, by comparing it with the Kurucz Solar Atlas, we will have SME solve for the optimal gf values to produce a better fit in Section 3.

1   Obtaining the Atomic Line Data

The Vienna Atomic Line Database (VALD) is a collection of atomic line parameters from theoretical and experimental sources. Making a request to VALD will return the best data available for each parameter. The data may be requested via either the e-mail service of the Web-based service. We will use the e-mail service here. You'll need to register in order to use these services, so be sure to sign up before hand. It may take a few days for VALD to establish your account. Further information on becoming a VALD client and the different procedures for data extraction is available on the web [2].

Once you're a client, make a VALD Request for a line list by sending the following (in the message body) to `vald@astro.univie.ac.at`:

```
begin request
extract stellar
default configuration
short format
5000.0000, 5005.0000
0.005,1.0
4000,4.44
end request
```

This request is for a line list for the solar chemical composition in the wavelength interval 5000.0-5005.0 Å, with microturbulance 1 km s^{-1}, and a detection limit of .5 % so that only lines that dip .5% or more below the continuum are retrieved. The temperature of the model is 4000 K with a log surface gravity of 4.44. Retrieving the data in VALD short format and the default configuration enables easy data input in SME.

It may take up to 30 minutes for VALD to send you the atomic data via e-mail. Once you receive this, save the data as a `.lin` file to your SME directory. Then use a text editor to remove all lines preceding the one with the starting and ending wavelengths. After doing this, the first line of the file should look like (for this example):

```
5000.0000, 5005.0000, 32, 153, 1.0, Wavelength region, lines selected,
lines processed, Vmicro
```

2   Generating the Synthetic Spectra

1. Start IDL and run SME from command line:

    ```
    bash>idl
    IDL>sme
    ```

    An **SME Tool** Widget window should appear.
    We can now compute synthetic spectra with SME. We begin by generating one with fixed values.

2. In **SME Tool**, click on **Line Data**.
   Select Line Data Files window appears.
   Select the line data file obtained in Step 1.
   Click **Ok** to close window (*Warning!: Do not, at any point during the use of the SME widget, close windows by clicking on the X-windows 'close window' button in the top corner*).

3. In **SME Tool**, click on **Controls**. Select **Global Parameters**.
   Global Parameters window appears.
   Enter the parameters.
   For the Sun, these are (remember to include the periods, and to hit carriage

return after each entry):

Teff:	5770.
Gravity:	4.44
[M/H]:	0.0
Vmicro:	1.0
Vmacro:	3.6
Vsini:	0.0
Vrad:	0.0
Cscale:	Each seg
G_6 Factor:	2.5

Click **Done** to close window.

4. Load the observed spectra by clicking on **Observations**.
   Choose Observations window appears. Select **Segment of an atlas file**.
   Select SME-Style Atlas File window appears.

   Look for Kurucz Atlas in /usr/local/sme/atlases/. Now, select the file describing a 'quiet' sun with a wavelength range for which the wavelength range we're modelling is a subset of. In our example, this is `qsun04999_06248.fits`.

   Click **Ok** to close **Choose Observations** window.
   Click **Done** to close **Select SME-Style Atlas File** window.

5. Click **Jobs**. Enter name for job in **Object Name** and hit RETURN. Check that parameters are set correctly by selecting **Review Current SME Request**. To compute the spectral synthesis, first save the request by pressing **Save Request**. This will create an SME input file with the name given in **Jobs**, and the suffix `.inp`. Now do **Submit SME batch job** to start the calculations running in the background. SME creates an output file and a log file at this point.

   When the computations are done, click **Done** to close **Jobs** window.

6. Now go to **Examine** and select **Read SME structure from disk**, and read in the output file (which has your job name plus the `.out` suffix). Do **Plot Flux Profiles** to display the spectra. You should now see three plots of the spectra corresponding to the starting systhesis, the final systhesis and the observations. These can be turned on or off by pressing the respective buttons on the control

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panel just above the plots. Note that the plot is colour-coded to show continuum points (light background) and line points (darker background). Across the top of the plot, there should be a series of labels identifying the chemical species of the lines and their wavelengths. These wavelength labels are each underlined to different degrees. The length of these lines correspond to the (relative) abundance of the element such that where there are two or three lines close together (a 'line blend'), the dominant line would be the one indicated with the longest underscore.

Close the plot by pressing **Close**.

3 Solving for gf values and Van Der Waals broadening

[1]

As seen above, the synthetic spectrum with default parameters does not fit the observed spectrum of the Sun very well, but by choosing certain parameters to be 'free', SME will be able to modify the spectra by tweaking these values to determine the best possible fit to the observed spectrum.

1. Try solving for the gf values by pressing the **log (gf)** button under **Controls/ Free Parameters**.
   Which log(gf) are free parameters window appears.
   Select two or three lines for whose $\log(gf)$ values you wish to solve, and make a note of their wavelengths. As long as the lines are not too close together (such as in the line blends) it is ok to solve for them simultaneously.

2. Submit a new request under **Jobs** to have SME generate a new spectra (see § 2, item number 5.). To see what adjustments SME made during the fitting iterations, choose **Examine** and **Print Free Parameters**. Is there a steady reduction in the χ^2 error with each iteration?

3. The fits may be improved even further by telling SME how to handle the different pixels in the observed spectrum. Read in either an input (`.inp`) or an output (`.out`) structure from disk (see § 2, item number 6). Plot the flux profiles and choose **Edit Mask**. You can now tell SME to omit certain points from the computation by selecting regions as "bad" by holding and dragging the right mouse button, or reinstate them as "good" with the left mouse button. The **Switch to line/cont** button toggles between allowing you to mark

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[1]see eg. Gray [3] Chapter 11 for more information on this

line or continuum regions (There is a slight idiosyncracy here, in that SME will only allow you to mark continuum points *after* they have been marked as "good" line points.). Now mark only the lines for which you want SME to solve the gf values (which you had noted down earlier) as "good" pixels, and anchor the simulation by choosing several continuum pixels spread uniformly over the whole plot.

Once you have edited the mask, click **Close** to close plot window.

Goto **Jobs**, provide a new name, and review the current request carefully for which parameters should be kept fixed and which should be determined via the fit procedure. Try again to solve for the gf values. How has the line profile changed in terms of depth or broadening?

4. At this point, you may be satisfied with the accuracy of some of the synthetic lines as compared with the observed spectra. Tell SME to stop solving for the gf values in these lines as follows. Choose **Show lines** in the control panel above the plot. A **Line info** window appears. Clicking on a line in the plot would update the contents of this window to reflect the information associated with that line. In particular, the **Solve** button next to **log gf** and **Gwaals** tells you if SME is solving for the gf values and the Van Der Waals broadening for that line. Turn off solving for gf values in your well-matched lines by unchecking the **Solve** box next to **log gf**.

In some of the other lines, however, you may find that just varying the gf values alone did not produce a good fit. Tell SME to solve for Van Der Waals broadening in the line *simultaneously* by checking the **Solve** box next to **Gwaals**.

Click on **Show line** again to close the sub-window.
Click on **Close** to close plots window.

Go to **Jobs**, provide a new name, and have SME solve for the spectra again. Compare your solution with the previous case and explain what happened [2].

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[2]Note that for lines deeper than a relative intensity of 60% (i.e. those that extend below the 0.4 mark on the ordinate) the solution is inaccurate as non-LTE effects are present for which the code does not take in to account.

4 Correcting wavelengths

You may have noticed that for some lines on the plot, the troughs don't quite correspond to the same wavelength. Correct this discrepancy between VALD data and the observations as follows. In the plots window, make a note of the wavelength of the line in the observed spectra by moving the cursor over to the line, and noting it's wavelength from the display in the control panel. Close plot window and **Results** window. In the **SME Tools** window, go to **Controls** then select **Line parameters**. A window displaying the VALD parameters for the lines in the model appears. Double-click on the element whose wavelength needs to be altered. The parameters for that line then appears in the edit boxes below the list. Change the wavelength here to the observation value you recorded earlier from the plot. Click **Update** to register these changes in the list above, and check that this is right.

Click **Done** to close **Line parameters** window.

Go to **Jobs** and run the computations again. Then bring up the plot to confirm the match.

This tutorial was modified and enhanced by K.L.Tah from the computer exercises by Eric Stempels [4].

References

[1] J. Valenti and N. Piskunov, Astron. Astrophys. Suppl. Ser. **118**, 595 (1996).

[2] http://www.astro.uu.se/~vald.

[3] D. F. Gray, *The Observations and Analysis of Stellar Photospheres* (Cambridge University Press, Cambridge, 1992).

[4] http://www.astro.uu.se/~mizuno/Atmos/lab2.pdf.