Synthetic meteor spectra

Introduction

Meteor spectra show prominent emission lines of Mg, Na, Fe and other elements from the meteor itself and from the terrestrial atmosphere such as O and N as well as molecular bands (the most prominent is the N2 ($B^3\Pi_g \rightarrow A^3\Sigma^+_u$) first positive band (Abe 2020). In order to learn about the composition of the meteor, it is common practice to measure line intensities from the different elements in order to determine element abundances in the meteor and also determine the temperature of the plasma which produces the optical emission. In low resolution spectra which will be treated here, the task is complicated by the fact that many meteor lines overlap and assignment to the different elements is not easy. In order to resolve this problem, synthetic meteor spectra are generated and adjusted to the measured spectra with a least square fit. From the fit parameters the line intensities of different elements can be extracted in an objective way. The calculations are integrated into the processing pipeline m_spec for the analysis of video meteor spectra (meteorspectroscopy.org/unified-python-script-for-calibration-and-processing-of-meteor-spectra). At the moment the script is still in an experimental stage, improvements are planned.

Generation of meteor spectra

When a meteor enters the terrestrial atmosphere, the meteor surface ablates and forms a plasma composed of meteor material and air. The recording and analysis of meteor spectra has been described before, here we concentrate on the calculation of synthetic meteor spectra. The ablation of the meteor is a complex process, we simplify it by assuming that we observe a plasma in thermal equilibrium at constant temperature. We also assume a low density plasma without self-absorption. Under these simplifying assumptions the intensity of a spectral line is given by the equation

$I_{ki} = N*g_k*E_{ki}*A_{ki}*\exp(-E_k/(k*T_{pl}))$ (1)

With the number density N of the atomic species for the transition of an upper level k and a lower level I ($g_k = 2*J_k + 1$ is the multiplicity of the upper level, E_{ki} and A_{ki} are the transition energy and transition probability of the spectral line and the exponential describes the population probability of the upper level at the assumed plasma temperature T_{pl}.

The data for these calculations are found at the NIST atomic spectra database:
https://physics.nist.gov/PhysRefData/ASD/lines_form.html

The data for the most relevant elements have been downloaded and are used for the spectral calculations. The equation (1) gives the relative intensities for all lines of a single atomic species. It can also be used to calculate the relative abundance of different atomic species, but this only gives correct results if the excitation corresponds to the assumed thermal equilibrium, which is hardly true for the ablation process. Nevertheless, the relative strength of the lines of different atomic species gives important information about the meteor ablation process. In addition to the atomic lines, meteor spectra also present molecular bands, in particular the first positive band of molecular nitrogen between 560 and 760 nm. Spectra for this molecular band have been created for different plasma temperatures with the program Pgopher (http://pgopher.chm.bris.ac.uk/index.html, described in Colin M. Western, N2 spectrum Arxiv1905.02528.pdf). In addition, blackbody radiation from the solid meteor is also observed. This continuum is described by the Planck function:

$I_{planck} = \text{const}/(\lambda\text{^}5 * (\exp(hc/k/lamda/temp) - 1))$ (2)

With λ in [nm] and hc/k = 14.3866e6 for T in [K]
(Gordon Walker, Astronomical observations, Cambridge University Press, 1987, reprinted 1999)

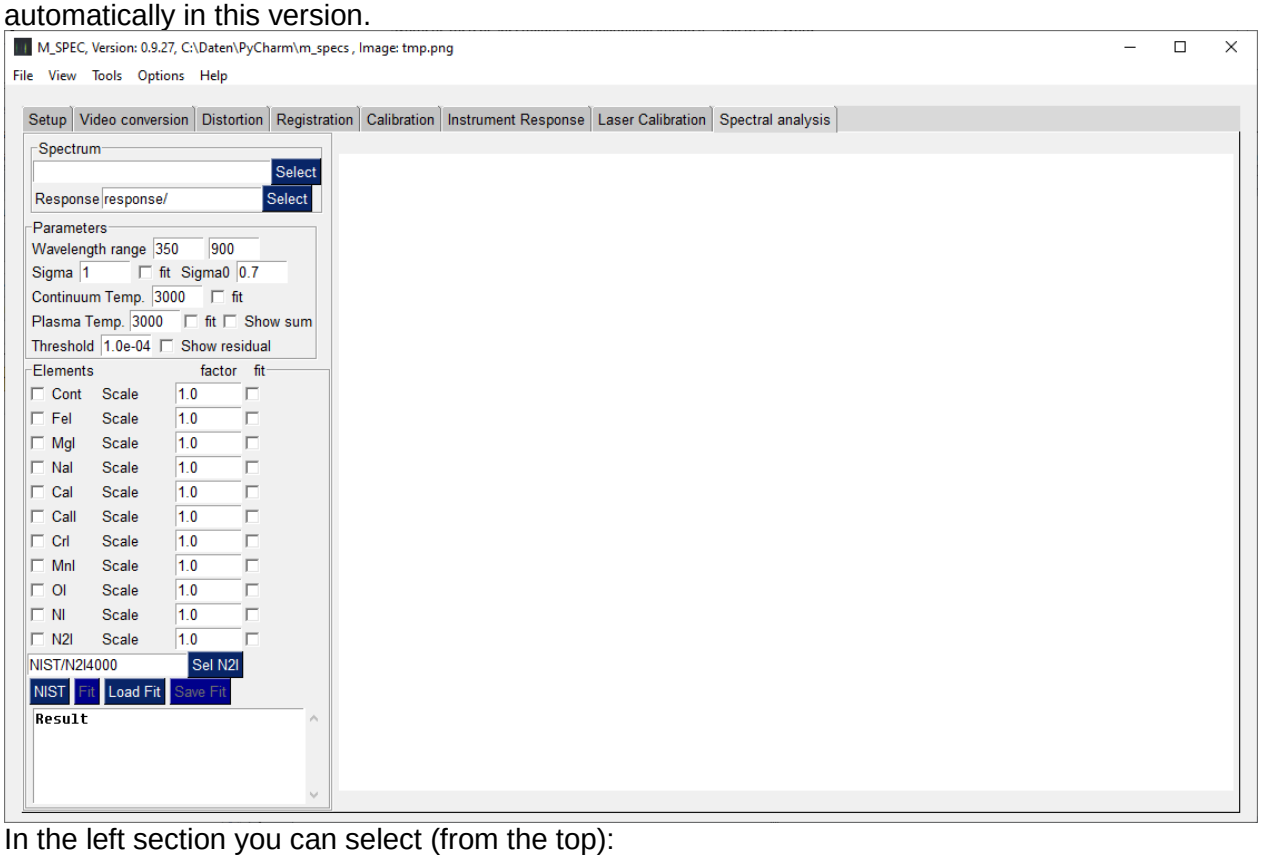
Comparison with observed meteor spectra

The observed meteor spectra are compared with the calculated meteor spectra. The amplitudes of the different atomic species, molecular nitrogen and the amplitude and temperature of the

continuum radiation are adjusted with a least square fit. The instrument response function has to be taken into account. There are two possibilities. The first method applies the instrument response function to the meteor spectra and adjusts the weight of the different spectral measurements according to the value of the response function (the measurements with lower sensitivity have lower weights). The second method, used here, multiplies the calculated spectrum with the response function and compares this spectrum with the measured spectrum directly, with equal weights for all measurements. By this method, measurements with low sensitivity are automatically weighted less.
Other parameters which can be adjusted by the least square fit are the instrumental resolution and the plasma temperature. The fit of the plasma temperature is rather slow, because all atomic spectra have to be recalculated, so it may be advisable to fit it in second step, after fitting the other parameters with a reasonable constant value. For the fit of the other parameters the spectra have to be calculated only once, the amplitudes can be adjusted with a linear least square fit.

Running an example

The script can be loaded from https://github.com/meteorspectroscopy/meteor-spectrum-calibration
Load the branch synthesis. It will be merged later into the main branch after some testing.
The synthetic spectra are calculated in the tab “Spectral analysis”, which is selected automatically in this version.



In the left section you can select (from the top):

- Meteor spectrum to be analysed (by default selected from a folder analysis, but this can be changed when desired)
- Instrument response function (by default selected from the folder response, but other files are allowed as well)

Several parameters for the fit, such as:

- Wavelength range. This is very important. The instrument response is normally defined only for the first order and usually for the visible range, therefore it is advisable to limit the wavelengths to a suitable range such as 400 to 800 nm. The fit is calculated only for this range, possibly further limited by the spectral range of the meteor spectrum. The

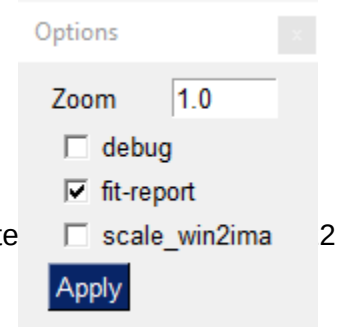
meteor spectrum also defines the wavelengths at which the synthetic spectra are calculated and the differences $I_{measured} - I_{fit}$, which are squared and summed for the determination of the least square fit.

- Instrument resolution. The line-shape of meteor spectral lines is approximated by a Gaussian profile with width parameter σ (approximately half width at half height, or more precisely FWHM = $2 * \sigma * \sqrt{(2*\ln(2))} = 2.3548 * \sigma$
(https://lmfit.github.io/lmfit-py/builtin_models.html)
$I = I0 * \exp(-(\lambda - \lambda_0)^2/\sigma^2/2)$
Since this parameter is adjustable, the synthetic spectra are first calculated with a smaller width σ_0, and for the fit of σ convolved with a Gaussian of width $\sigma_{fit} = \sqrt{(\sigma^2 - \sigma_0^2)}$. This saves computer time for the fit. Both the initial value of σ and σ_0 can be chosen. In order to give a reasonable fit, σ_0 should be chosen larger than 3x the sampling interval of the spectrum. If this is larger than the measured width σ of the meteor spectrum, the spectrum should be resampled with a smaller sampling interval before analysing it with this script (this could be built into the script, but has not been necessary so far).
- Temperature of the continuum [K]
- Plasma temperature [K]
- A threshold can be set to eliminate very weak transitions (scaled to the most prominent transition) in order to speed up the calculation. The default value is a good compromise between speed and accuracy.
- Finally the different spectra of continuum, atomic spectra and molecular nitrogen can be selected individually. The atomic spectra tables are stored in a folder \NIST and contain:
ritz_wl_air(nm) Aki(s^-1) Acc Ei(eV) Ek(eV) g_i g_k Type
  - wavelength [nm]
  - transition strength[s^{-1}]
  - accuracy
  - upper level energy [eV]
  - lower level energy [eV]
  - g_i and g_k (multiplicity)
  - type

  With the check-box at left you can include the element in the analysis, the scale indicates the computed scaling of the intensities to full scale, the factor multiplies the full scale intensity to the desired value and with the check-box at right you select the intensity for fitting.
  For the molecular nitrogen band you can select from different plasma temperatures.

For all the elements you can select the intensities manually. The largest intensity is always scaled to the full scale at linewidth σ_0. The checkboxes to the right of the elements and also to the right of sigma, continuum temperature and plasma temperature allow a fit of these parameters. For a start do **not** fit the plasma temperature. It is very slow and the results are only reliable under certain conditions, when sufficient lines of different upper level energies are visible. This part of the fitting is in an experimental stage, do not use it unless you know what you are doing.
Below this element selection box there are several buttons for the calculation of the synthetic spectra.

- With the button “NIST” you load the selected spectral data of the elements and calculate the spectrum for the desired plasma temperature and instrumental line-width. Before you can do this you have to load a spectrum and the instrumental response if available. After this initial calculation the next button “Fit” turns green. After a change of selected elements or plasma temperature the button turns blue or inactive, with “NIST” the new calculation is prepared.
- With the button “Fit” you do the least square fit. The Python module lmfit with the function minimize is used for that (https://lmfit.github.io/lmfit-py/fitting.html. The Levenberg-Marquardt method is used by default, which is useful for

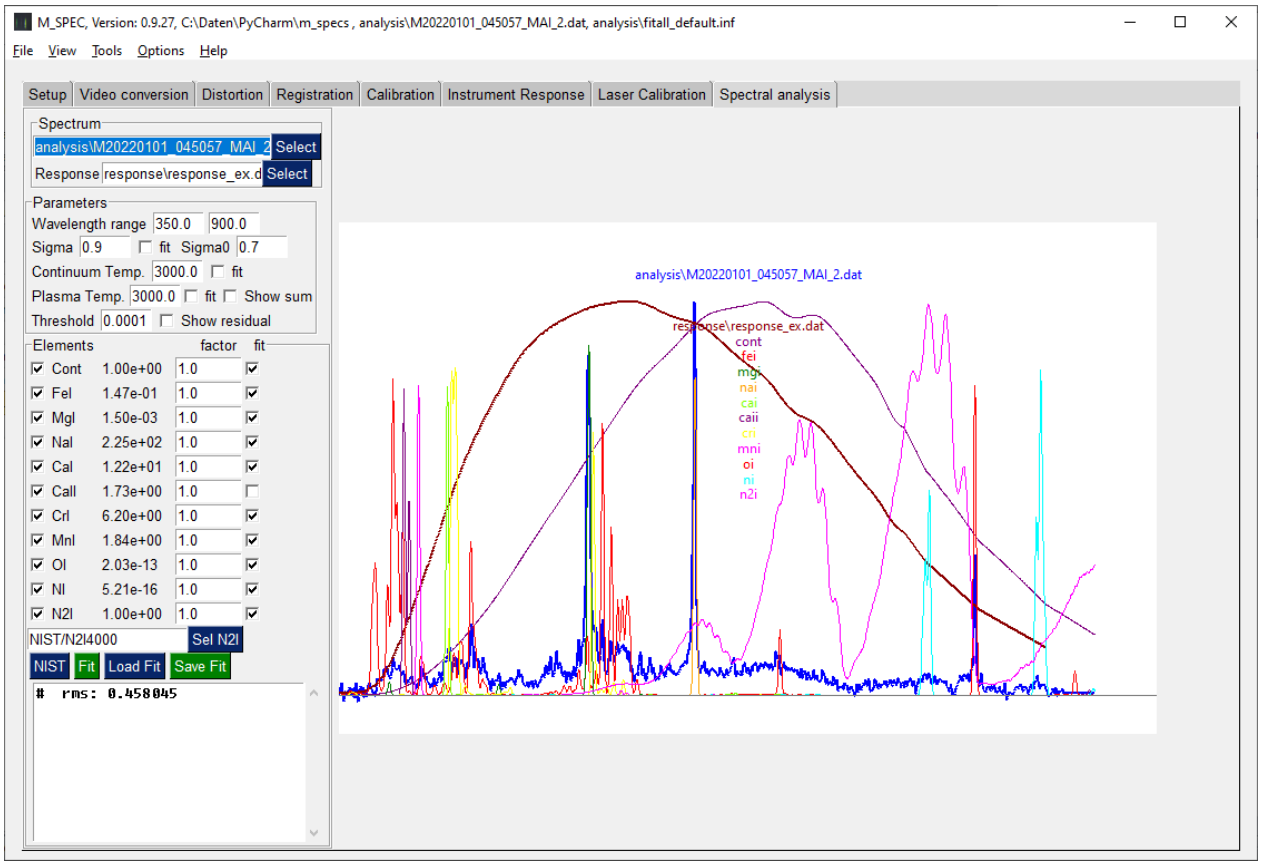


both linear and non-linear fits. If you are interested in the detailed results, you can select fit-report in the Options menu:
This prints a detailed fit-report in the Python window, showing different fit results such as correlations between fitting parameters.

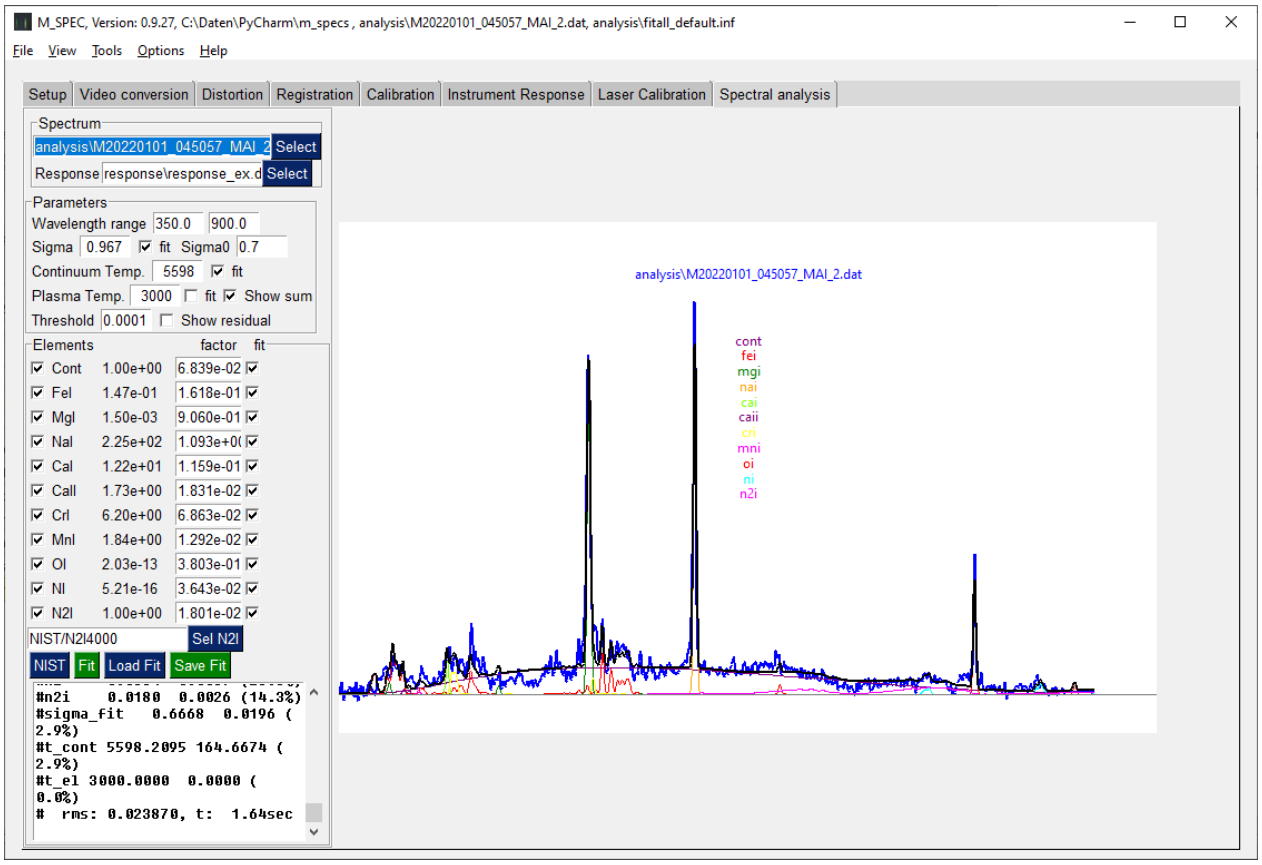
- Instead of selecting the different elements, continuum temperature and plasma temperature you may load an existing configuration with “Load Fit”, e.g. default_fit.inf. The appendix .inf denotes a fit configuration with preselected parameters including meteor spectrum, response, wavelength range, temperatures and linewidth σ, as well as selection of elements and intensities.
- Finally there is a button “Save fit”, which allows to save the current configuration (only active after the initial calculation with NIST has been done). It saves all the parameters in a file named by default *spectrum*_fit.inf (where *spectrum* denotes the name of the meteor spectrum), together with a calculated spectrum *spectrum*_fit.dat, which can be used for example for plotting or further analysis. You may also use this saved configuration as a template for another meteor spectrum, with good starting values for σ and temperatures, which speeds up the following calculations.

Least square fit

After you have loaded a spectrum, selected a response function, set the parameters to reasonable values, selected the desired elements and done the initial calculation with NIST you are ready for the least square fit. You may also try out a default configuration for a start, e.g. fitall3000default.inf:



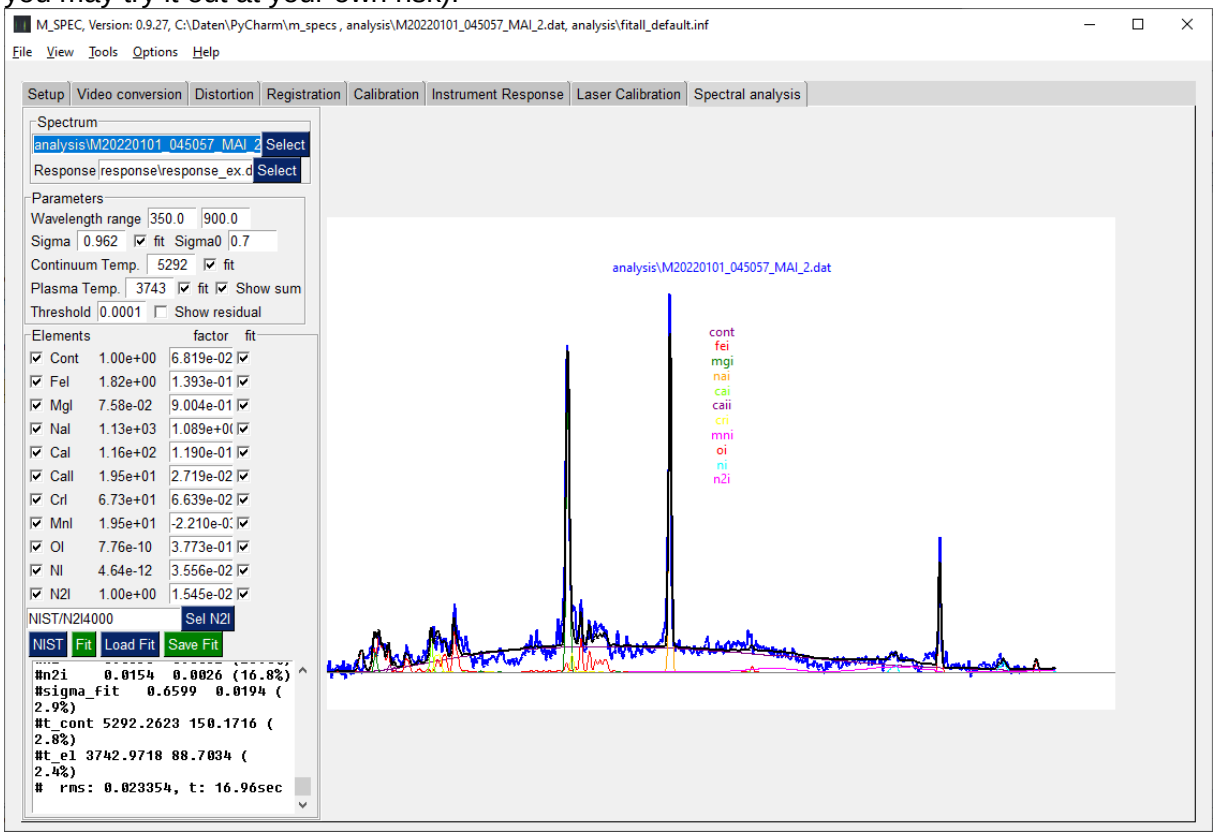
The fit adjusts line-width, continuum temperature, continuum and line intensities:



In the box at lower left the results of the fit are shown with some details (values and errors of the different fit parameters and the rms-error of the final fit

rms = sqrt[$\Sigma_k(I(\lambda_k) - I_{fit}(\lambda_k)^2/(N_k - N_f)$]

An additional fit of plasma temperature reduces the rms-error further (does not always work, but you may try it out at your own risk):



In this case the results for the continuum temperature and plasma temperature have reasonable values, the Mg and Na-lines are fitted well, not all Fe-lines have the correct intensity, an indication that the condition of thermal equilibrium is not well satisfied.
Parameters with negative values you may choose to set to zero and do not fit, also values with large errors.
A word of caution:
Minimizing the rms-error does not mean that the results are correct, it only means that the solution reduces the error, but does not indicate whether the result is physically meaningful.

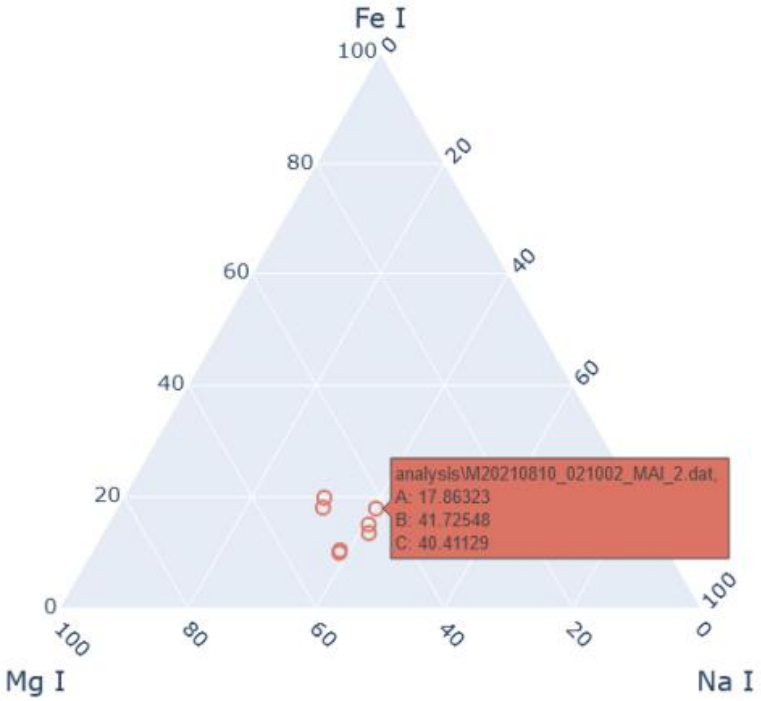
Zoom view for details

The wavelength and amplitude scale of the graph does not show small details such aas overlapping lines or line-shapes. In order to show that, a zoom feature has been added to the graph synthetic spectra. Zoom by drawing rectangle (with left button down) from left to right, up or down. Reset zoom by drawing rectangle from right to left.

You can also measure wavelength and intensity by clicking into the plot, results are shown in the window title as x = … y = … Useful for measuring line positions, especially when zoomed in

Presentation of results

The resolution of the present spectra is not quite sufficient to determine quantitative contributions of all elements, since the spectra of different species partially overlap. However it is possible to determine the main elements Fe, Mg and Na. This is often used in practice to classify meteor spectra into distinct groups (Borowicka, 2005), (Matlovic, 2019). By this method, 3 prominent line groups of Fe I – 15 (523 -550 nm), Mg I – 2 (512 – 523 nm) and Na I – 1 (584 - 594 nm) are compared. Their intensity is measured by integrating the fitted line profile of these elements over the indicated wavelength ranges. This has the advantage that the continuous background and overlapping line of other elements can be eliminated. The choice of these line groups has an additional advantage. They are fairly close together near the maximum sensitivity of most detectors. Therefore small variations in the instrument response and atmospheric absorption have little influence on the ratio of these intensities. The result is typically plotted as a ternary diagram, which gives the relative intensities normalized to the sum in a triangular diagram, with a pure Fe spectrum located at the top, a pure Mg spectrum located at the bottom left and a pure Na spectrum at the bottom right:



The example shows the result of different meteor spectra recorded last year contained as examples in the folder \analysis. The diagram was produced with a small python script extracting the fit results from the logfile and plotting them as a ternary diagram with the help of Plotly: https://plotly.com/python/ternary-plots/
This result shows one application of the present analysis program. Other applications are the time dependent evolution of these element ratios and the application to different meteor streams.
Plotly is installed with `conda install -c conda-forge plotly`

References

Abe, 2020:
Shinsuke Abe et.al., Sodium variation in Geminid meteoroids from (3200) Phaethon, Planetary and Space Science 194 (2020) 105040

NIST atomic lines database: https://physics.nist.gov/PhysRefData/ASD/lines_form.html

Pgopher: http://pgopher.chm.bris.ac.uk/index.html,
described in Colin M. Western, N2 spectrum, Arxiv1905.02528.pdf.

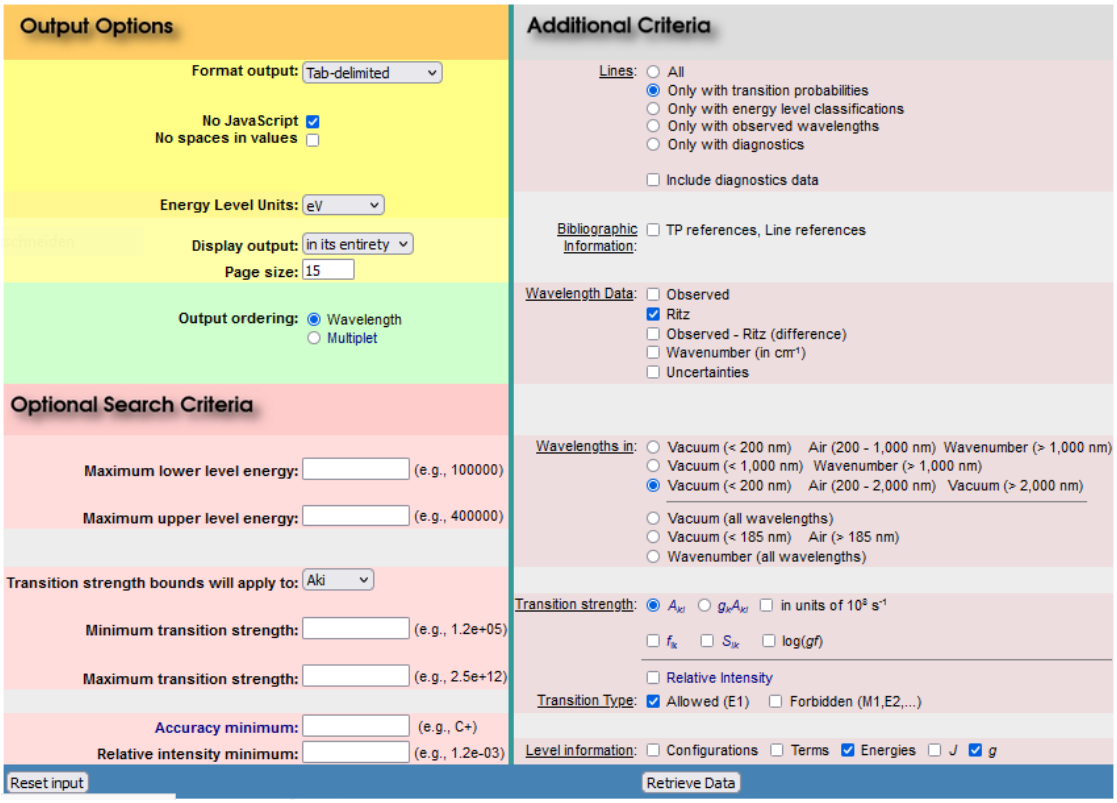
Borowicka, 2005:
J. Borovicka , P. Koten, P. Spurný, J. Bocek, R. Štork, A survey of meteor spectra and orbits: evidence for three populations of Na-free meteoroids, Icarus 174 (2005) 15–30

Matlovic, 2019:
Pavol Matlovic, Juraj Tóth, Regina Rudawska, Leonard Kornoš, and Adriana Pisarcíková ˇ, Spectral and orbital survey of medium-sized meteoroids, arXiv:1908.01565v2

Appendix

Adding elements to the database

In case you would like to add other elements, it is important that the data files (FeI.txt etc.) are in the correct format. This is done with the following settings in the NIST database (https://physics.nist.gov/PhysRefData/ASD/lines_form.html):



(no relative intensities, no forbidden transitions, no J, wavelength ordering)
You can ignore it, if you use just the script as is with the following elements:
`'Cont', 'FeI', 'MgI', 'NaI', 'CaI', 'CaII', 'CrI', 'MnI', 'OI', 'NI', 'N2I'`

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