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DEVELOPMENT OF A SOFTWARE FOR INAA ANALYSIS AUTOMATION

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ABSTRACT

In this work, a software to automate the post-counting tasks in comparative INAA has been developed that aims to become more flexible than the available options, integrating itself with some of the routines currently in use in the IPEN Activation Analysis Laboratory and allowing the user to choose between a fully-automatic analysis or an Excel-oriented one. The software makes use of the Genie 2000 data importing and analysis routines and stores each "energy-counts-uncertainty" table as a separate ASCII file that can be used later on if required by the analyst. Moreover, it generates an Excel-compatible CSV (comma separated values) file with only the relevant results from the analyses for each sample or comparator, as well as the results of the concentration calculations and the results obtained with four different statistical tools (unweighted average, weighted average, normalized residuals and Rajeval technique), allowing the analyst to double-check the results. Finally, a "summary" CSV file is also produced, with the final concentration results obtained for each element in each sample.

1. INTRODUCTION

Instrumental Neutron Activation Analysis (INAA) is an analytical technique where samples are irradiated under a neutron flux and the induced activity is then used to determine the concentrations of several elements in the sample at once. When the comparative variation of INAA is used, as is the case in the in Neutron Activation Analysis Laboratory of IPEN (LAN/IPEN), the samples – in a typical case, several samples at once – are irradiated together with comparators with well-determined elemental composition, which can be either elemental standards or certificate reference materials (CRMs), so that the elemental composition of the samples are then determined by comparing the induced activity in the samples and comparators.

The post-irradiation processes involved in such an experiment include the analysis of several gamma-ray spectra, the identification of the gamma-ray lines of interest to the calculations in each of them and the calculation of the concentrations by comparing the results for each gamma-ray in the sample and in the comparators. Moreover, if more than one gamma-ray line can be used to determine the concentration of a given element, or if that given element is found in more than one comparator, some sort of statistical treatment shall be performed to result in a more reliable final result, possibly with a lower uncertainty [1]. All these tasks can be either carried out individually (i.e., the spectra

analysis and the concentration calculations are performed separately) or as a single task, using one software to perform the analysis and the calculations automatically.

In LAN/IPEN, there are a few choices for each of the two main processes. The analysis of the gamma-ray spectra can be performed either using the in-house developed software VISPECT (or the Python version of the same algorythm, embedded in the SAANI package [2]) or the Canberra Genie 2000 software [3], which seems to be a better alternative according to a recent evaluation [5]. As for the concentration calculations, they can be performed automatically using either the Genie 2000 NAA package (which only works in systems where Genie 2000 performs the data acquisition as well, as the software controls both the data acquisition and analysis) or the SAANI package, or manually, where the results are printed then typed in either an in-house developed software or an Excel spreadsheet. Despite the many advantages of the automated analysis, most of the samples are still analyzed manually, due to limitations or lack of transparency in the automated software, or to the steep learning curve associated with them.

The aim of this work was to develop a software to automate all the post-counting tasks which:

- Can deal with spectra originated in any of the different acquisition systems available in LAN/IPEN;
- Allows the user to double check the results by outputting to the user not only the final results, but also the intermediate ones;
- Has a modular design, so that some of the tasks may be performed by different sotware and/or methods, in order to allow the user to adapt it to his needs or preferences;
- Whenever possible, employs robust statistic techniques to ouput the best possible results from the experimental data.

2. COMPARATIVE INAA PROCEDURE

In a Comparative INAA measurement, it is usual to irradiate several samples at one, together with a few comparators; the full procedure, then, comprises several individual tasks:

1. Samples and standards preparation;
2. Irradiation (usually in a nuclear rector);
3. Gamma counting;
4. Gamma spectra analysis;
5. Comparison of the induced activity in the samples and standards;

6. Compilation of the individual results for each element to reach a final concentration value for each sample.

Tasks 1-2 are mechanical and, therefore, out of the scope of this work. For the remaining, post-irradiation tasks, most of the work is performed in a computer environment, and there are a few software or procedural choices for each of these tasks. The next sections will deal briefly with the choices and particularities of each of these steps, as well as present the solutions chosen and/or developed in this work.

2.1. Gamma Counting

The counting of the gamma-ray activity in the samples and standards is performed using high-resolution HPGe detectors, which are coupled to some sort of digitizer that will build an histogram of counts as a function of pulse height (which is assumed to be proportional to the gamma-ray energy) [4]. These interfaces are mostly proprietary, so that the counting task has usually to be performed using a software distributed by the digitizer's manufacturer, so the resulting output file is also of a fixed format. In the LAN-IPEN facilities, the digitizers are all made by either Canberra or Ortec and the acquisition software available are Ortec's Maestro or Canberra's S-100 and Genie 2000; the output spectra are then either in Ortec's CHN format or in Canberra's MCA or CNF formats.

2.2. Gamma spectra analysis

The analysis of the gamma-ray spectra is, arguably, the most important and sensitive of the post-irradiation tasks. A typical gamma-ray spectrum has something like a hundred peaks, together with their Compton borders, a background, and many other deleterial effects. There are many software solutions to this task; in LAN-IPEN, for instance, two solutions are frequantly used: VISPECT, a DOS-based application developed in-house that outputs a printed list of transitions and their respective counts and uncertainties; and Genie 2000, a MS-Windows-based program that may produce the same output either to a printout or to an ASCII file.

A recent comparison of spectrum-fitting software showed that Canberra's Genie 2000 software delivers good spectrum analysis results [5]; two additional advantages of Genie 2000 are that it can import data in several formats (including CHN and MCA) and that it can be fully operated by the command line, making it an ideal choice to deal with the spectrum analysis task in an external software. Therefore, the choice in the present software implementation was to use Genie 2000 to perform the analysis os the gamma-ray spectra; nevertheless, the software was clearly divided in two main components, one which uses Genie 2000 to analyse the spectra and another which reads the results of this analysis and processes them – this option was made so as to make it rather trivial to couple some other spectrum analysis software's output to its input.

2.3. Comparison of the Induced Activity in the Samples and Standards

This task is rather straightforward, comprising the identification of the gamma-ray energies associated with each isotope of interest and the calculation of the concentration of the correspondent element by the simple equation 1:

$$C_s = C_c \cdot \frac{A_s}{A_c} \cdot e^{-\lambda \cdot dt} \tag{1}$$

where the subscripts s and c refer to the sample and comparator, respectively, C is the element's concentration, A is the net area of the respective gamma-ray peak, λ the decay constant of the radioactive isotope and dt the time elapsed between counting the sample and the comparator.

While the decay of some isotopes produce a single gamma-ray transition, in some cases there are several (even hundreds) of them. The usual procedure in LAN-IPEN is to print the results of the gamma-ray spectrum analysis and then type them either in another in-house DOS-based software (ESPECTRO) or in some MS-Excel spreadsheet. This procedure is both time-consumming (between printing and retyping the results, this procedure may take 5 minutes or even more for each sample) and may introduce errors, as typographical mistakes could happen.

In the present software implementation, the data from the spectrum analysis software is automatically imported to the calculus software, and the choice of transitions to be used is defined in an external file, so that the final decision is then left to the user. In all the results presented throughout this work, though, the transitions suggested by Bode [6] are employed, following also the conclusions of a previous work [1].

2.4. Compilation of the Individual Results

In the end of a typical Comparative INAA measurement, the analyst may be presented with an array of concentration results for the same element in the same sample – for instance, if a given element is associated with three gamma-ray transitions and is found in three different comparators, the analyst will have up to 9 individual results for that element's concentration in the sample. In a recent work [1], the problem of reaching the most precise and exact final value (with its associated uncertainty) was studied and the conclusion was that, when more than three individual values were present, the use of a robust approach such as the Normalized Residuals Mean (NR) or the Rajeval Technique Mean (RT) gives the most reliable final result, with the lowest feasible uncertainty. The present software calculates both these means, together with the traditional unweighted and σ^{-2}-weighted averages, and delivers all these results to the analyst.

3. CURRENT AUTOMATED ANALYSIS SOFTWARE OPTIONS

Presently, there are two choices in LAN-IPEN for automated experiment analysis: Canberra's NAA package and the in-house developed SAANI [2], but for one reason or another neither or them are suitable for all the analysts' needs.

3.1. Canberra NAA

The Canberra NAA package is a collection of routines written in the REXX. REXX is an interpreted copmputer language, meaning that the interpreter must be installed in the computer that will run the software. Also, the NAA package was written with the whole process in mind, as it takes care of both the gamma-ray counting and of the subsequent tasks – it does not calculate any kind of average, though, and its documentation is basically unexistent, so that the fine details of the calculations made are hard to determine, and any personalization of the software is rather hard to do and time-consumming. Also, the package depends on the presence of the Genie 2000 software, which will do the data acquisition and spectrum analysis.

Due to these limitations, the NAA package is of limited use in LAN-IPEN, both because it can only be used in systems where Genie 2000 is installed and coupled to the detector to be used and because there is too little space for customization, so that even small changes required by some experiment are very hard to implement.

3.2. SAANI

The SAANI package [2] was developed with the aim of taking care of all the post-counting tasks. It was written in Python, which is also an interpreted language and thus require the interpreter to be installed on the system, too. One additional problem is that it has no support for the (proprietary) Canberra CNF spectrum format used by Genie 2000, so that in order to be used with data acquired with Genie 2000 a third-party converter (for instance, Cambio [7]) has to be used. The spectrum analysis routine implemented is simply a port of the VISPECT routine (originally written in Basic) to the Python language, which proved to be rather error-prone [5]. The most serious issues with SAANI, though, are limitations in the definition of the standards (or comparators), together with the interface, which proved to be a bit too unintuitive for most analysts. As a consequence, SAANI's use in LAN-IPEN has never really taken off.

4. DESCRIPTION OF THE SOFTWARE

The software was developed using the Pascal computer language, which is compiled and has free, open-source compilers for most of the operating systems available [8] – this way the software itself is comprised of a batch of standalone executable files which, with a single exception, do not require any additional software to run properly; furthermore, the compiled code is small (not more than 1MB) and is capable of running properly in a variety of host systems (tests up to now include Windows 98, XP and 7, both 32 and 64 bits).

4.1. Gamma Spectra Analysis

This is the only task that requires some additional software, as the analysis is, at this point, made by Canberra's Genie 2000 software (which runs fine in Windows XP and 7 – 32 bits only – but requires a separated licence and a hardware key to work). Basically, the present software works as follows:

- Finds all spectrum files in the current folder (presently, the CHN, MCA and CNF extensions are looked for, but the list could be easily increased);
- Converts the non-native formats to Genie 2000's CNF format (using Genie 2000's "filecnvt" command);
- If instructed by a command-line option, looks for a previously-calibrated CNF file previously saved in the software's "cal" subfolder and copies its calibration to the files to be analysed (using Genie 2000's "movedata" command);
- Runs Genie 2000's "analyze" command in each file, saving the report file (one for each spectrum) in the same folder as the spectrum files are located.

The report files are simple, plain-text space-delimited ASCII files which contain a header with information such as spectrum name and path, date and time that the data acquisition started and real and live times of counting; also, it includes a list of the gamma peaks found, with the corresponding Energy (in keV), Resolution (also in keV), BG counts, Liquid counts per second, 1σ uncertainties (in %) and centroid channel. In fact, the use of a different software for the spectrum fitting task would be straightforward, provided that it delivers a similar output for each analysis.

4.2. Calculations

For the calculations to be performed, some additional information has to be entered, such as the identification of the samples, the names of the files related to the first and (optionally) second counting of the samples, masses and, in the case of standards, a description of the standard – the time that the acquisition took place is obtained automatically from the report files. In the case of the standards, a description file must be stored in the software's "padroes" subfolder; this file (also a plain-text space-delimited ASCII file) contains informations as the "name" of the standard (for reporting purposes) and one line for each gamma-ray line to be analysed with the following information: symbol of the element, gamma-ray energy (in keV), decay constant (in min^{-1}), concentration, uncertainty and in which counting this energy should be verified (1st, 2nd, or both).

With all this information, the software then performs the following tasks:

- Reads the report files for each sample or standard, storing the time information (both start time and counting realtime, so that to calculate the mid-time and use it as "spectrum time" to correct for the decay while counting);

- For each report file, identifies it as first or second counting and looks for the transitions to be analysed in that counting, storing the results (energy, counts per second and uncertainty) – the "tolerance" (in keV) for gamma-ray identification defaults to 2keV, but can be set in 1/10's of keV using a command-line option;
- For each sample, calculates the concentrations obtained using each transition (using eq. 1), for each comparator where that transition was found and the element's concentration has been defined[1] – this way, many different concentration results may be stored for each element in each sample;
- If more than one result was obtained for a given element's concentration in a sample, calculates the arythmetic and σ^{-2}-weighted means;
- If more than two results were obtained for a given element in a sample, calculates the Normalized Residuals and Rajeval averages;
- Outputs one ASCII report file for each sample with, for each element and transition, the results of the individual calculations, as well as the decay constant and peak areas (to allow for a double-check, if desired);
- Outputs an ASCII file where the results are grouped by sample, with the individual concentration values for each element for each transition/standard/counting set, together with the averages for that element in that sample;
- Outputs a CSV (comma-separated values) file, readable by a regular spreadsheet software, with the final results and uncertainties for the concentrations of all elements and samples (the presented values are the Normalized Residuals mean, when 3 or more results are present; the weighted average, when 2 results are available, or the single result, if that's the case).

The two robust averages are calculated using the instructions found in the papers where they were proposed: Normalized Residuals [9] and Rajeval [10].

5. EXPERIMENTAL PERFORMANCE

The software was tested in data from five separate measurements from the LAN-IPEN group, all in soil samples. In all the measurements, the SRM's IWG-GIT BE-N (Basalt), NIST 8704 BRS (Buffalo River Sediment) and ANRT GS-N (Granite) were used as comparators so, in order to check the performance of the software when compared to the manual analysis, the BE-N standard was treated as an unknown sample, both using the software and the manual procedure, and the concentration values were calculated and compared to the certificate for each of the five measurements. In all cases, 25 elements were included in the analysis: As, Ba, Ca, Ce, Co, Cr, Cs, Eu, Fe, Hf, K, La, Lu, Na, Nd, Sb, Sc, Sm, Ta, Tb, Th, U, Yb, Zn, and Zr. In the software analysis, the result used for each element was:

[1] If the transition is marked to be analysed in both countings, both values will be calculated independently, too

- Rajeval average, if 3 or more results were present;
- Weighted average, if 2 results were present; and
- The single result, when only one was present.

As for the manual procedure, the analysis was a bit trickier, performed by an experienced analyst the way it is usually done in the present day, so the result used was:

- The weighted average, when all the results for an element were compatible;
- The unweighted average (and the standard deviation) when the results were rather compatible (i.e., the standard deviation was larger than the weighted average's uncertainty, but less than 3 times this uncertainty);
- The single result with the lowest relative uncertainty, provided that the obvious outliers were removed, when the results were incompatible.

When only two absolutely incompatible results were present and had a similar relative uncertainty, the unweighted average and the standard deviation were used.

Finally, for each measurement the zeta-score (eq. 2) and the relative uncertainty (eq. 3) were calculated for all the elements found, and the result are presented in table 1. Basically, the results can be summarized as follows:

- The software only failed to determine the concentration of an element once (K in the 5th measurement), whereas the manual analysis failed to determine K in the 1st, 3rs and 5th measurements, Th in the 1st and 5th measurements, and Cs, Zn and Zr in the 4th.
- The software gave results with a Zeta-Score greater than 3 only for Nd, in the 2nd and 5th measurements, whereas the manual analysis resulted in Zeta-Scores greater than 3 for Cs in the 1st and 5th measurements, for Fe in the 2nd and 4th measurements, and for K in the 2nd measurement.
- In general, the software delivered uncertainties that were lower, or of the same magnitude, of the uncertaintied obtained in the manual analysis; some remarkable exceptions, though, were Eu in the 1st measurement, As in the 3rd measurement, Sb in the 3rd and 5th measurement, and U in the 5th measurement.

$$Z_i = \frac{x_i - x_{ref}}{\sqrt{\sigma_i^2 + \sigma_{ref}^2}} \tag{2}$$

Table 1: Results of the analysis of the IWG-GIT BE-N (Basalt) certified reference material in 5 separate measurements, using both the manual procedure and the software.

Elem	CERT.	I1				I2				I3				I4				I5			
	VAL.	MANUAL		SOFTWARE		MANUAL		SOFTWARE		MANUAL		SOFTWARE		MANUAL		SOFTWARE		MANUAL		SOFTWARE	
	($\mu g.g^{-1}$)	Z	RU(%)	Z	RU(%)	Z	RU(%)	Z	RU(%)	Z	RU(%)	Z	RU(%)	Z	RU(%)	Z	RU(%)	Z	RU(%)	Z	RU(%)
As	1.80 (3)	-1.0	33.4	0.0	16.7	-0.2	28.4	1.7	16.0	0.4	37.8	-0.6	100.0	1.0	21.8	-0.4	9.2	-1.0	33.4	0.0	27.8
Ba	1025 (30)	-0.4	4.0	-1.5	4.0	-2.1	4.3	0.6	3.0	-0.6	3.6	-1.7	3.4	-0.9	4.4	-1.0	6.3	-0.4	4.0	-0.3	4.2
Ca*	9.92 (16)	2.3	18.2	-0.4	7.3	-1.8	10.0	1.2	6.5	1.2	10.4	-2.0	6.9	-0.7	14.8	-1.0	7.6	2.3	18.2	-1.3	7.8
Ce	152 (4)	-0.5	5.3	-0.7	5.5	0.0	5.3	-0.3	5.4	-0.7	5.2	-0.7	5.5	-1.0	5.3	-1.0	4.9	-0.5	5.3	-0.7	5.5
Co	60 (2)	-0.1	2.6	0.1	2.7	0.0	2.6	0.0	2.5	-0.1	2.6	-0.1	2.5	-1.2	2.6	-1.1	2.6	-0.1	2.6	0.2	2.6
Cr	360 (12)	1.4	3.4	1.2	3.4	1.7	3.4	1.4	3.4	0.2	13.4	1.3	3.4	-0.9	3.4	-1.1	3.5	0.1	15.1	0.0	3.6
Cs	0.80 (10)	-3.9	52.7	-0.5	27.1	-2.9	48.8	-1.8	12.1	0.2	16.9	-1.1	17.5			0.1	24.4	-3.9	52.7	0.1	18.5
Eu	3.60 (18)	-2.0	2.9	0.8	5.7	1.1	18.8	0.6	3.5	0.9	19.7	0.1	2.5	0.3	8.9	0.7	5.8	-0.7	12.8	0.7	3.2
Fe*	8.98 (4)	1.1	0.9	1.5	0.8	3.0	0.9	2.9	0.8	1.6	0.9	2.0	0.8	-3.2	0.9	-2.7	1.2	1.2	1.4	2.7	0.9
Hf	5.60 (16)	-0.8	5.7	-2.1	4.0	-0.2	5.8	-0.8	3.9	0.0	5.6	-1.4	3.8	-0.8	6.1	-1.4	4.0	-0.8	5.7	0.1	4.1
K*	1.15 (2)			-0.4	25.0	-3.3	51.2	-0.5	30.0			-1.6	35.1	-1.9	21.3	-2.0	17.6				
La	82.0 (15)	1.7	2.6	1.6	1.9	-2.9	0.9	1.9	1.9	0.8	2.6	1.2	1.8	0.0	2.6	-0.1	1.8	1.7	2.6	1.3	1.9
Lu	0.24 (3)	-0.9	11.1	-0.3	11.8	-0.4	11.2	-0.5	11.3	-1.1	10.7	-0.8	10.5	0.3	11.3	-0.5	12.3	-0.9	11.1	0.1	11.1
Na*	2.36 (3)	-0.4	6.9	-0.2	1.3	-0.3	7.2	0.0	1.3	-0.5	8.1	-0.5	1.3	-0.9	7.0	-2.1	1.3	-0.4	6.9	0.5	1.3
Nd	67.0 (15)	-1.4	3.2	2.4	4.0	-0.2	4.0	-3.3	2.5	-1.5	6.2	-2.4	3.5	0.0	4.5	0.2	7.4	-1.8	3.9	-4.6	3.6
Sb	0.26 (5)	0.1	18.5	-0.9	14.3	-0.8	26.7	-0.6	18.2	-1.4	25.4	-1.9	100.0	-0.1	20.6	0.6	35.3	0.1	18.5	-0.5	100.0
Sc	22.0 (15)	0.6	5.5	0.6	3.9	0.9	5.5	1.0	3.8	0.7	5.5	0.7	3.9	0.2	5.5	0.2	4.0	0.6	5.5	0.9	3.8
Sm	12.2 (3)	-1.1	3.0	-0.9	2.5	-0.4	3.0	-0.9	2.5	-1.1	3.0	-1.9	2.6	-1.8	3.0	-0.6	3.4	-1.1	3.0	1.0	3.1
Ta	5.7 (4)	-0.7	62.1	-0.4	7.3	0.5	9.9	0.5	6.7	0.2	6.1	0.7	6.6	0.9	7.4	0.2	6.9	-0.7	62.1	1.9	7.2
Tb	1.3 (1)	-0.7	13.3	-2.4	6.9	0.1	13.9	1.5	7.8	-0.1	12.3	-0.7	6.6	0.1	20.3	-2.8	11.1	-0.7	13.3	-0.5	6.5
Th	10.4 (7)			-0.2	8.8	0.5	8.6	0.4	8.3	-0.4	8.6	-0.6	8.2	-0.7	8.7	-0.6	8.2			0.1	8.6
U	2.40 (18)	0.9	9.5	2.5	7.1	1.0	13.3	0.6	7.4	0.4	43.0	-0.4	8.7	0.4	45.8	-0.6	7.1	0.9	9.5	0.2	44.4
Yb	1.8 (2)	0.2	12.3	-0.3	8.7	-0.3	19.0	0.2	7.1	-0.4	7.4	0.1	6.6	-0.6	9.3	-1.2	8.6	0.2	12.3	-1.6	8.5
Zn	120 (13)	-0.2	20.6	0.7	3.1	-0.5	4.5	0.6	3.1	0.6	83.9	1.0	3.0			0.1	4.1	-0.2	20.6	1.0	4.5
Zr	260 (10)	0.5	18.7	1.4	22.7	-2.2	13.9	0.8	24.9	-0.3	11.0	-2.5	13.0			-2.8	31.2	0.5	18.7	0.4	14.4

* Values in %.

$$RU_i = \sigma_i / x_i \tag{3}$$

In general, the use of the Genie 2000 software for fitting the spectra, instead of the VISPECT, proved to give more consistent results, with the individual concentration values for each element in each sample being a lot more compatible with each other. Also, the use of a larger set of transitions and of a robust averaging technique delivered more reliable results, most of the time with a lower uncertainty.

Finally, the Genie-2000 peak fitting procedure proved to be the most time-consumming part of the analysis – it took approximately 3.5 seconds to analyse each spectrum in a 700MHz Pentium III and 2.5 seconds in a 2.2GHz Celeron 450; the time required to perform all the remaining calculations was less than a second (for a whole batch) even in the Pentium III. As a comparison, the analysis of the same amount of data by the "manual" method required something like 30 minutes for a single sample with two comparators – the time for a usual measurement with approximately 10 samples and 3 comparators, thus, may add up to more than 2 hours, compared to less than 5 minutes using the software.

6. PERSPECTIVES FOR FUTURE ENHANCEMENTS

The software is still under development and undergoing several tests, so there are quite a few features that will hopefully be added to it in a near future.

The first one is the ability to do a "quick recalibration" for each spectrum, based on the list of peaks actually found and their expected energies, according to the standard definition files; performing a simple linear regression and recalculating the energies for all peaks present in the spectrum report file would allow a second peak identification to be performed, with a much lower tolerance, so as to avoid the misidentification of peaks.

Another feature that should be implemented, based on the first tests, is the ability to manually remove one or more values and recalculate the robust averages – at this point this can be made by manually eliminating the corresponding line from the spectrum fit results (the "rpt" file) or by removing the corresponding line from the comparator definition file (in this case, though, the results related to that transition / comparator pair will be removed from the analysis of all the samples in that batch).

Finally, some sort of graphical user interface (GUI) should be developed to assist the user in the tasks of creating the experiment definitions, the definitions of the standards, as well as in running the software as a whole.

7. CONCLUSIONS

The software was developed with the aim of assisting the users in the process of comparative NAA data analysis, and proved to deliver consistent and reliable results, requiring

just a small fraction of the time it would take to undergo the traditional, "manual" procedure. The software permormed well, finding more elements than the manual procedure, as well as delivering more reliable results, often with a lower uncertainty.

The aim now is to enhance the software usability for non-technical users, as well as to introduce a few enhancements that shall make the results even more robust and allow more user control of the final calculations (for instance, allowing the user to simply remove a spurious result from the final calculations).

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