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CAX A SOFTWARE FOR AUTOMATED SPECTRUM ANALYSIS

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ABSTRACT

In this work, the scripting capabilities of Genie-2000 were used to develop a software that automatically analyses all spectrum files in either Ortec's CHN or Canberra's MCA or CNF formats in a folder, generating two output files: a print-ready text file (.DAT) and a Comma-Separated Values (.CSV) file which can be easily imported in any major spreadsheet software. This software, named CAX ("**C**onvert and **A**nalyse for e**X**cel"), uses Genie-2000's functions to import spectrum files into Genie's native CNF format and analyze the converted spectra. The software can also, if requested, import energy and FWHM calibrations from a stored calibrated spectrum.

The print-ready output file (.DAT) is generated by Genie-2000 using a customized script, and the CSV file is generated by a custom-built DAT2CSV software which generates a CSV file that complies to the Brazilian standards, with commas as a decimal indicator and semicolons as field separators. This software is already used in the daily routines in IPEN's Neutron Activation Laboratory, greatly reducing the time required for sample analyses, as well as reducing the possibility of transcription errors.

1. INTRODUCTION

The analysis of gamma-ray spectra is a key part in any application involving gamma-ray spectrometry, and there is plenty of software to choose from to perform this task [1]. These software usually perform a set of functions: read the spectrum file; import or adjust the energy – and, sometimes, FWHM – calibration; locate the gamma-ray peaks in the spectrum; determine the precise location, width and area of each peak; output the results.

While seemingly simple, many of these tasks differ strongly from software to software. Some software, for instance, can only import spectra in a very narrow selection of formats – if the software also controls the data acquisition, it may import only its own native format. Also, most acquisition software can only export spectra in its native format, and that changes from time to time, even for the same manufacturer. Thus, in a laboratory that has equipment from more than one manufacturer, and of distinct age, it is not uncommon to have to deal daily with 3 or 4 distinct spectrum formats, increasing the importance of using a single platform that can import spectra in many different formats.

Also, the results from these fits will most likely be used as input for further data analysis, so it is important that the output can be easily integrated in the next steps of the analysis.

In this point, also, software may differ greatly, either outputting the results directly to a printer (usual in the most ancient software), to a regular output file, or even be very customizable, accepting custom report formats.

Finally, regarding the spectrum analysis process, software may also differ greatly. Some may offer a possibility to perform energy and FWHM (Full Width at Half Maximum, a measure of the system's energy resolution) calibration, other may only import the calibrations from the spectrum file, and HypermetPC even performs its FWHM calibration "on the fly" [2]. The quality of the peak-finding and fitting routines is also very variable, as shown by the authors in a previous study [1].

This way, in order to simplify and unify the spectrum analysis process in a complex laboratory with several different detectors and diverse possibilities of data analyses, it is essential to choose a software that can both read spectra in different formats and output the results in an easy-to-use format.

1.1. Genie-2000

Canberra's Genie-2000 software [3] is very flexible in its use. While it only works with its native .CNF format, it is capable of importing all of the most common spectrum file formats. Moreover, the spectrum analysis and results reporting stages are all greatly customizable by means of user-editable analysis scripts (.ASF) and report templates (.TPL).

Another important feature is that Genie-2000 has a modular built, with a main Graphical User Interface (GUI) as a front-end for easy interactive operation, but most complex internal operations being performed by standalone command-line programs [3], allowing for an easy, seamless integration of some third-party software [4].

Taking into account that Genie-2000 has also been shown to deliver reliable spectrum analysis results [1], it was chosen as the basis for an automated spectrum analysis software for daily use at IPEN's Neutron Activation Laboratory.

2. SOFTWARE DESIGN

The software, named CAX (acronym for "**C**onvert and **A**nalyze for e**X**cel"), was written in the Pascal language and compiled using the open-source FreePascal compiler [5]. Although FreePascal is available for many platforms, so that CAX might be ported to all of those, the software makes use of many of Genie-2000's executables, which run only under 32-bit Windows – another very important limitation is that it will only run in systems with a working registered version of Genie-2000.

2.1. Syntax

At this time, CAX will run exclusively in command-line mode, fitting all the spectra found in the current folder using the same settings. The syntax is:

```
CAX [/N] [/L] [Calibration File]
```

where exactly one of the parameters must be used. "/N" tells CAX to use the internal calibrations found in the spectrum file itself (i.e., no recalibration whatsoever); "/L" lists all calibration files found in the calibrations folder (at present this is not configurable, and all calibrations are expected to be found at the `c:\aan\cal\` folder); and "Calibration File" is the name of the calibration file to use.

The command will result in the creation of two ASCII report files for each spectrum file in the folder, a printable one with the ".RPT" extension and an excel-compatible one with the ".CSV" extension. Also, if the original spectrum was not in the .CNF format, a CNF file will be created.

2.2. Importing Spectra

In the first step of the software execution, it locates all spectrum files within the current folder, using Pascal's *FindFirst* function – as these are the only formats used in our laboratory, it actually searches only for .CHN, .MCA and .CNF files. If any report files are found in the folder, the software automatically creates a backup folder with the current date and time as name, to avoid overwriting previous backups, and moves the reports to that folder. After that, the software run all its commands for each spectrum file, before moving to the next.

In the next stage, the software runs `filecnvt`, a tool available within Genie-2000's executables folder which imports the spectrum file into its native .CNF format.

2.3. Importing Calibrations

Genie-2000 offers an executable called `movedata`, which is intended to copy parts of a spectrum file into another; as the calibrations are among the parts it can copy, if requested the CAX software then runs this command with the following parameters: `/overwrite /ecal`, which means that *a* if there is a corresponding section in the spectrum file, it will be overwritten; and *b* that the section to be copied is the energy calibration (which includes FWHM calibration, too).

The energy calibration files are regular .CNF files with proper energy calibration, one per spectrometer, which are stores in a specific sub-folder of the CAX folder (at the present time, rigorously `c:\aan\cal\`).

2.4. Analyzing Spectra and Reporting Results

This stage, which is the core of the software, also makes use of a Genie-2000 executable file, `analyze`. This tool performs the peak finding and fitting, and also creates a report.

The analysis part requires a specific "Analysis Sequence" script with the .ASF extension, created inside the main Genie-2000 GUI. This script contains the sequence of steps to be run at the analysis stage and their options – in this case, peak finding, with the proper

settings, and peak fitting, also with a set of parameters; these settings and parameters may depend on the laboratory's specific demands, but using Genie's default options is generally a good starting point. Moreover, the script also contains a section to inform what media to report to (on-screen, printer or file), which sections of the report to output (these are defined in the .TPL file), as well as the exact formatting of the report – which is defined in a separate template file, with the ".TPL" extension.

In the present case, a customized version of this template file is used, which reports the name of the input spectrum file, date/time and both real and live time of acquisition, followed by a list of peaks, one by line, with peak number (just used as a reference), Energy (in keV), Resolution (keV), BG (total continuum counts under the peak), CPS (net count rate, in Counts Per Second), 1-sigma uncertainty for the count rate (in percentage), and the channel of the peak's centroid (used to check calibrations in the laboratory's daily routine).

The regular ".RPT" Genie-2000 report uses international number conventions (with dots as decimal separators), which unfortunately don't apply to the default installation of most spreadsheet software (including the ubiquitous Microsoft Excel®) in Brazil, where commas are used as decimal separators. To ensure an easier and more transparent use, CAX then runs its own simple external file converter (`RPT2CSVBR`, also written in Pascal), which reads the report file, replacing dots with commas and blank spaces with semicolons (with an additional step to make sure that sequential spaces are treated as a single one), so that the output file conforms to the Brazilian CSV (Comma Separated Values) standard, where commas are decimal separators and semicolons are used to separate fields.

3. CONCLUSIONS

Although it runs only in command-mode, in computers where Genie-2000 is properly installed, the CAX software is already being used in the daily routine of many users in IPEN's Neutron Activation Laboratory. The main advantages of its use are the increased analysis speed and the ease with which the reports can be imported in spreadsheets for the calculation of concentrations, avoiding the need to retype the results of the peak analysis manually; as a bonus, the software has also served as an incentive for users to keep their spectrum files, which previously were frequently discarded after fitting.

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