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DEVELOPMENT OF A GAMMA RAY SPECTROMETRY SOFTWARE FOR NEUTRON ACTIVATION ANALYSIS USING THE OPEN SOURCE CONCEPT

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ABSTRACT

In this work, a new software – SAANI (Instrumental Neutron Activation Analysis Software) was developed and used for gamma ray spectra analysis in the Neutron Activation Laboratory (LAN) of the Nuclear and Energetic Research Institute (IPEN-CNEN/SP). The software was developed to completely replace the old one – VISPECT. Besides the visual improvement in the user interface, the new software will allow the standardization of several procedures which are done nowadays in several different ways by each researcher, avoiding intermediate steps in the calculations. By using a modern programming language – Python, together with the graphical library Qt (by Trolltech), both multi-platform, the new software is able to run in Windows, Linux and other platforms. In addition to this, the new software has being designed to be extensible through plug-ins. In order to achieve the proposed initial scope, that is, completely replace the old software, SAANI has undergone several and different kinds of tests, using spectra from certified reference materials, standards and common spectra already analyzed by other software or that were used in international inter-comparisons. The results obtained by SAANI in all tests were considered very good. Some small discrepancies were found and after careful search and analysis, their source was identified as being an accuracy bug in the old software. Usability and robustness tests were conducted by installing SAANI in several laboratory computers and following them during daily utilization. The results of these tests also indicated that SAANI was ready to be used by all researchers in the LAN-IPEN.

1. INTRODUCTION

The method of Neutron Activation Analysis (NAA) is known for its sensitivity for the detection and determination of a large number of chemical elements. The method consists of the production of artificial radionuclides from stable elements by irradiation of a sample in a neutron flux and measuring the radiation emitted by radionuclides formed in the process[3].

The Neutron Activation Laboratory (LAN) of the Nuclear and Energetic Research Institute (LAN-IPEN) uses the comparative method of instrumental neutron activation analysis, where sample and standards are irradiated together under the same conditions of irradiation time and neutron flux. The concentration of a particular element is obtained by comparing the counting rates of sample and standard spectra, obtained from the same counting geometry conditions.

The spectra analysis is done using a series of routines to locate and quantify the peaks, obtaining several data such as: peak energy, peak net area, peak background area, detector

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energy resolution, median channel, initial channel, peak width in number of channels, activities in counts/seconds and its standard deviation. These calculations are performed for all spectra of the sample and standard, after which the concentration results are obtained.

There are several software for the analysis of data from gamma spectroscopy [2]. Some are commercially available, some are freely available and some are distributed with the manufacturer's spectroscopy equipment.

Among the several software are: GammaVision-32 made by Ortec [5], Genie-2000, made by the Canberra [1], Hypermet-PC made by the Institute of Isotopes, Budapest, Hungary and HyperLab [7]. These softwares are distributed in the form of "closed executable code", that is, new features can't be freely developed and incorporated for them or even they can't be easily integrated with other software for the expansion of its capabilities.

The present paper describe the software developed, its main features, some of the software engineering techniques used in its development, a few comparison between the old software and SAANI as well as the tests that were conducted in order to validate the results obtained with the new software SAANI.

2. SOFTWARE DEVELOPMENT

2.1. Software engineering procedures

The survey of requirements for the development of SAANI was conducted through interviews and meetings with the LAN staff and also through a detailed study of Vispect software, whose source code, in BASIC programming language, was available. Vispect was developed by Dr. Denis Piccot, from the Pierre Sue Laboratory in Saclay site of French Atomic Energy Commission (CEA).

In the technical specification of the system, we adopted models based on UML - Unified Modeling Language. The UML has been adopted as standard for viewing, documenting and building artifacts of object oriented systems and can be used in all steps along the cycle of development [4].

The diagram of use cases, shown in Figure 1, helps to identify and specify the main system features, as proposed by the users.

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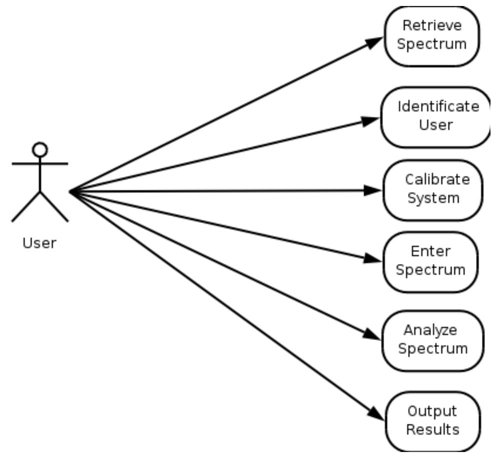

Figure 1. Use Cases.

SAANI has been modeled with seven classes; two of them are focused directly on business and a third class is used to provide access to spectrum data:

- Class LerEspectro: This class is responsible for reading the spectrum data from a disk file; upon success, a dictionary with the data - the values of counts for each channel, the file name read and other information is returned.
- Class QtBlissGraph: This class is responsible for presenting the spectrum plot on the screen and all the routines that involve its manipulation, such as the selection of a part of the graph to zoom (Zoom).
- Class VispectFit: This class is responsible for the search of spectrum peaks and to calculate their areas and also to deal, in some cases, with duplets. The following results are generated: peak energy, peak net area, peak background area, detector energy resolution, median channel, initial channel, width of peak in number of channels, activities in counts/second and its standard deviation.

2.2. Implementation

For the implementation of the software, aiming to create a free software with the object oriented methodology, the Python programming language was used. Python is a multi-platform language, object oriented, easy to learn but still powerful in its features. The graphical library chosen was QT, which can be used with Python by means of the PyQt binding[6].

QT is a multi-platform graphics library with an excellent performance, very powerful, with many resources for the development of graphical user interface. Trolltech, the company responsible for QT, released the version 4 of the library under the GPL license on all supported platforms, including from this version, the Windows platform [8], which was used for the development of all the graphical interface.

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3. RESULTS

As the proposed scope for SAANI was to completely replace VISPECT, a comparison between their user interface as well as some SAANI unique features are shown below.

3.1. Comparison between the user interfaces of software VISPECT / VERSION 2 and SAANI

The file opening screen for VISPECT is shown in Figure 2a and for SAANI in Figure 2b. As can be seen, the VISPECT interface has limited resources for the user, while the SAANI interface, using all the resources of the QT graphics library and modern operating systems is able to offer superior capabilities to the user.

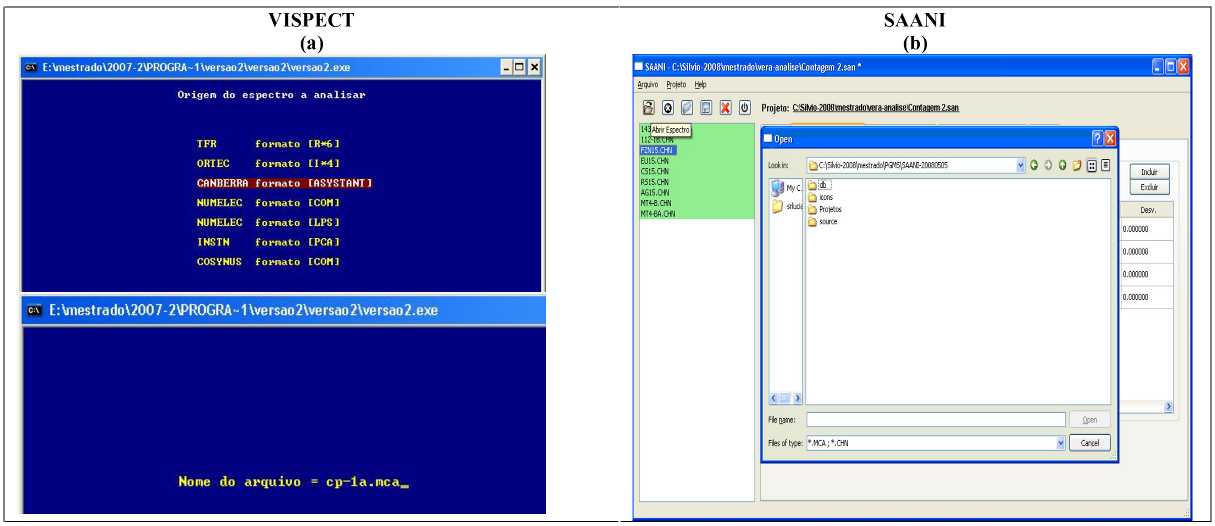

Figure 2. Main Screen option to open the spectrum file

The screens of the spectrum plot in VISPECT is shown in Figure 3a and for SAANI in Figure 3b. The interface of VISPECT provides limited resources to the user, while SAANI allows better visualization and greater flexibility in the inspection of the spectrum.

In the VISPECT software, to zoom in a spectrum region, the user has to use keys F2 and F3 to select the region and F5 to apply the zoom. The graphic routines implemented in SAANI, on the other hand, facilitate the identification and enlargement of the peaks in the spectrum in a fast, simple and easy way; by using the mouse and picking up a region, this is immediately zoomed to inspection.

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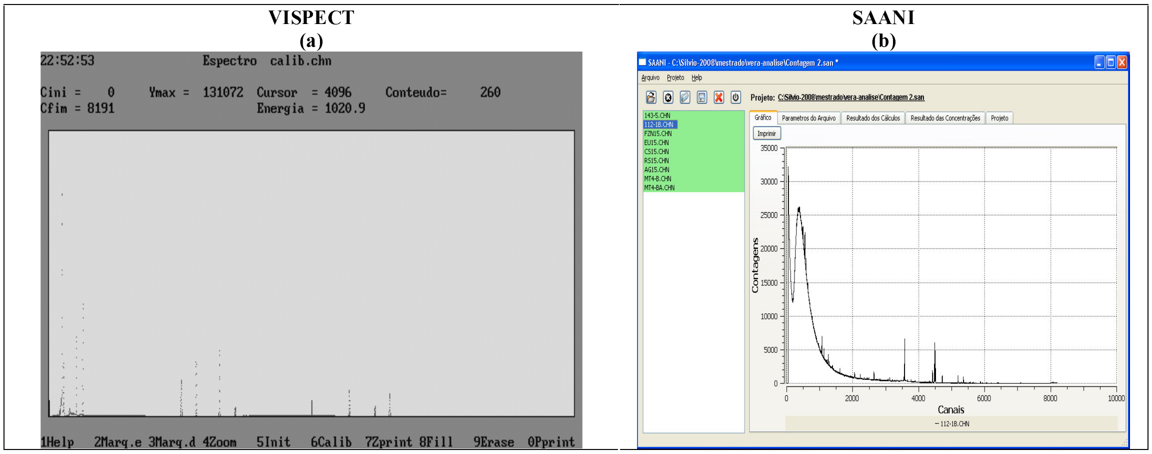

Figure 3. Spectrum plot

VISPECT does not perform the calculation of concentrations; these values are obtained in another software (e.g., a spreadsheet), by manually entering the output data from the printed report emitted by VISPECT and performing the calculations.

The new software - SAANI has the concentration routines integrated, eliminating separated calculations. For this, additional information about the standard or reference material, such as elements that are present and their respective concentration, date and time of the counting are required, as shown in Figure 4a.

The data analysis results in VISPECT are presented only in printed report form, while in SAANI they are presented on the screen, allowing the printing, if necessary, as shown in Figure 4b.

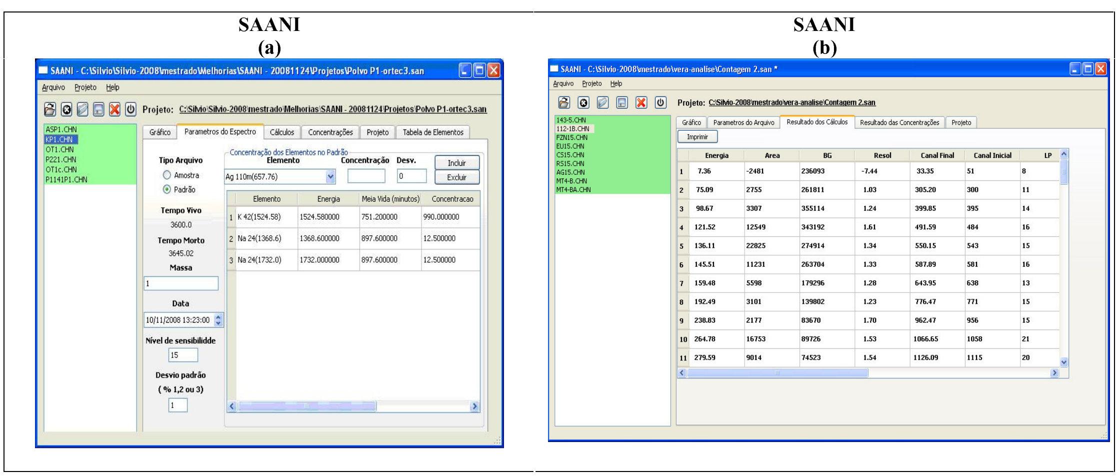

Figure 4. Additional Information Input Screen and Results

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3.2. Results of spectra analysis

For purposes of comparison and certification of the calculations made by the new software SAANI, several spectra were processed in VISPECT as well as in SAANI.

In this work the results of analyzing the spectra from two samples "112-1B.CHN" and "MT4-B.CHN" are presented, which were chosen because they offer good amount of items for comparison. In the Tables 1 and 2 are presented the results of net peak area determination made by the two softwares, where the excellent agreement of values obtained can be observed, except for the Se-75 lines (Sample 112-1B). The small difference in values for this element is due to a arithmetic bug in the VISPECT software, due to misuse of a single-precision number; in SAANI double precision number are used.

Table 1. Results of calculations made by the two softwares for Sample: 112-1B

Sample: 112-1B	Area			Activity (CPS)		
Elements	Vispect/ Versão 2	SAANI	Difference (%)	Vispect/ Versão 2	SAANI	Difference (%)
Eu-152(121,8)	12549	12549	0	0,349	0,349	0
Se-75 (136,01)	22825	22825	0	0,634	0,634	0
SC-47 (159,4)	5598	5598	0	0,156	0,156	0
Se-75 (264,66)	16753	16753	0	0,465	0,465	0
Cr-51(320,08)	3357	3357	0	0,093	0,093	0
Eu-152(344,3)	3001	3001	0	0,083	0,083	0
Se-75 (400,7)	4328	4520	4,25	0,120	0,126	4,76
Cs-134(604,7)	1501	1501	0	0,042	0,042	0

Table 2. Results of calculations made by the two softwares for Standard: MT4-B

Standard: MT4-B	Area			Activity (CPS)		
Elements	Vispect/ Versão 2	SAANI	Difference (%)	Vispect/ Versão 2	SAANI	Difference (%)
Eu-152(121,8)	3322	3322	0	0,092	0,092	0
Se-75 (136,01)	9259	9259	0	0,257	0,257	0
SC-47 (159,4)	10531	10531	0	0,293	0,293	0
Se-75 (264,66)	7469	7469	0	0,207	0,207	0
Cr-51(320,08)	1671	1671	0	0,046	0,046	0
Se-75 (400,7)	2081	2081	0	0,058	0,058	0
Cs-134(604,7)	531	531	0	0,015	0,015	0

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3.2.2. Results of the calculation of concentrations

One of the procedures used for concentration determination by the researchers of LAN-IPEN, is by the use of spreadsheets, where the appropriated formulas are already present, and the values are fed manually from the VISPECT reports.

For comparison with the SAANI, data from the VISPECT were fed in the Excel spreadsheet and compared with those obtained directly by SAANI; the results are presented in Table 3. The good agreement between the results can be observed, with most differences being less than 1.15%. Again, the Se-75 line shows the largest discrepancy, due to the error of accuracy mentioned above.

Table 3. Comparison of calculation result of the Concentration

Standard: 112-1B						
Elements	Concentration			Standard Deviation		
Standard: MT4-B	Excel	SAANI	Difference (%)	Excel 1s(%)	SAANI 1s(%)	Difference (%)
Se-75 (136,01)	3,92	3,92	0	0,42	0,42	0
Se-75 (264,66)	3,57	3,56	0,28	0,35	0,35	0
Cr-51(320,08)	0,88	0,87	1,15	0,31	0,31	0
Se-75 (400,7)	3,29	3,45	4,64	0,44	0,46	4,35
Sc-46(889,28)	0,18	0,18	0	0,01	0,01	0
Rb-86(1076,6)	4,33	4,30	0,7	0,28	0,28	0
Fe-59(1099,25)	581,00	581,07	0,01	21,78	21,66	0,55

4. CONCLUSIONS

The purpose of this work was to develop a free software for the gamma spectroscopy analysis performed by LAN-IPEN.

The goal originally proposed was reached, incorporating the otherwise separated procedures: to obtain the results of VISPECT software (peak energies, peak net areas, etc) and the determination of concentrations in one software.

To certify the results obtained by SAANI, several tests were carried out in which data analysis results for both softwares were compared. Concentrations results for VISPECT were, in fact, obtained by the conventional procedure used in LAN-IPEN (through spreadsheets), while for SAANI they were directly obtained. The comparison results demonstrated that SAANI implementation was accomplished with great accuracy, being trustworthy. This process of certification of the results is supported by the fact that VISPECT has been used by LAN-IPEN in programs of laboratory inter-comparisons, and its results have been validated in such programs[9].

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