



Peak identification in EDS Measurements using multiple subset sum problem formulation

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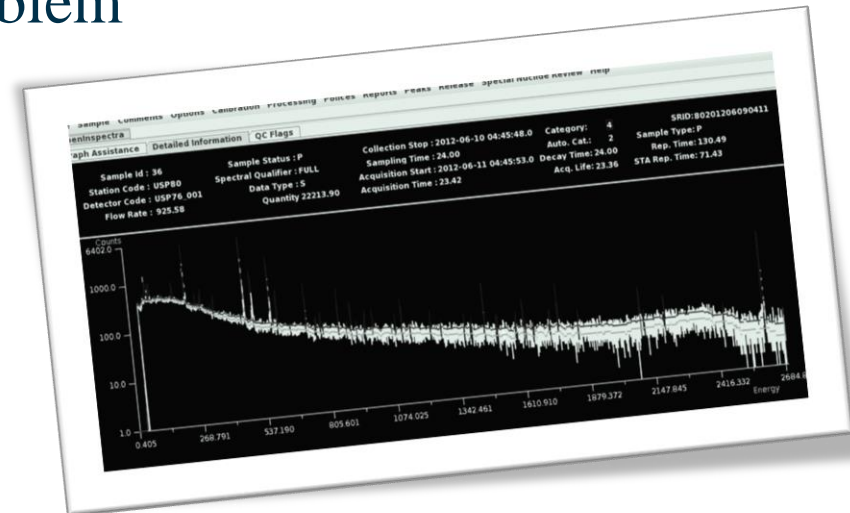
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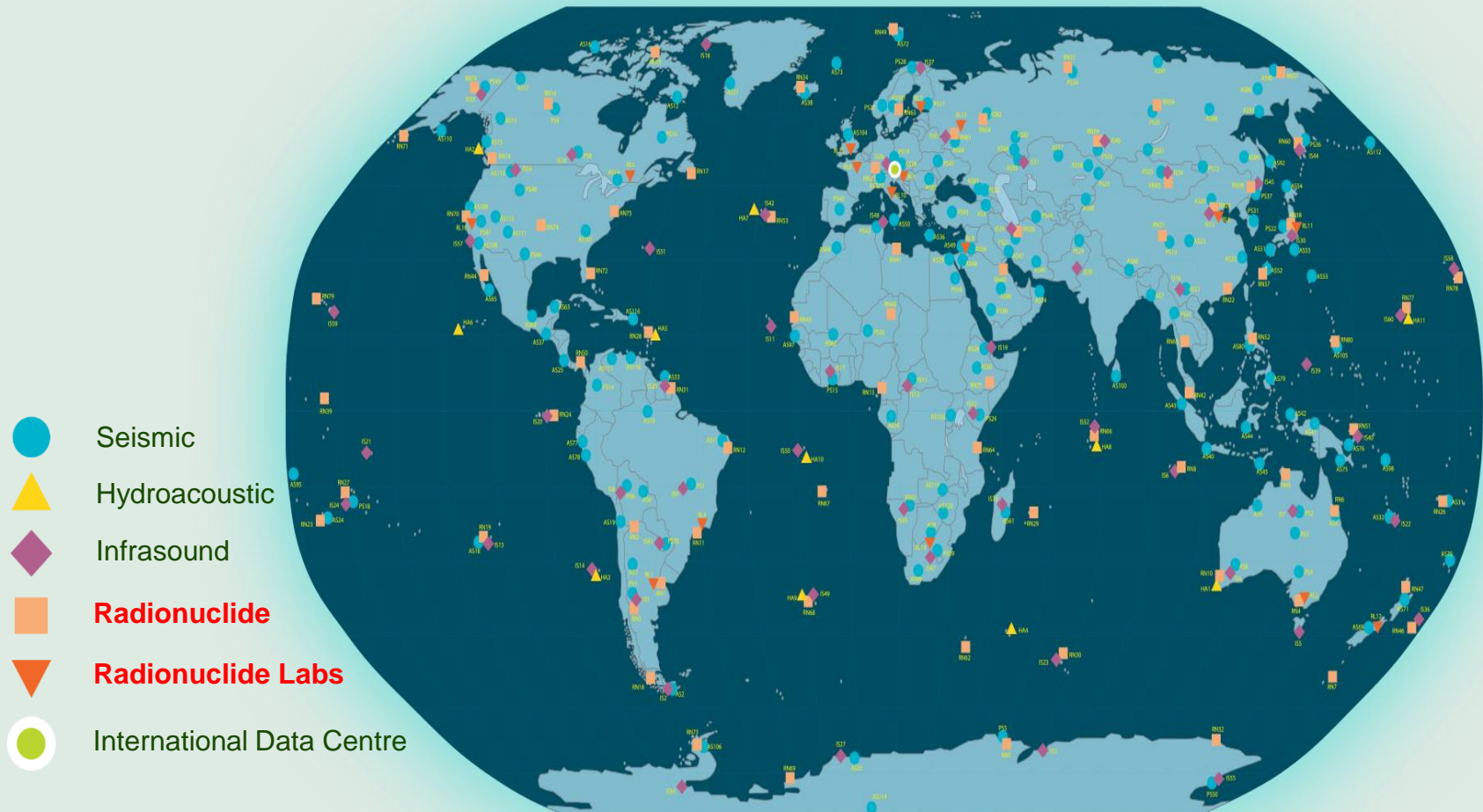
- Context and Background
- Subset-Sum Problem - SSP
- Gamma Spectrometry
- Unassociated Peak Vs Radionuclide
- Solving the Peak identification Problem
- Summary



- In the CTBT context, an “**event**” is any physical occurrence that is registered by the International Monitoring System, be it
 - ✓ *a natural or a man made event,*
 - ✓ *an earthquake or an explosion,*
 - ✓ *a chemical or a nuclear explosion.*

With regards to determining the nature of an event, Members States make the final judgement.

International Monitoring System: 337 Facilities

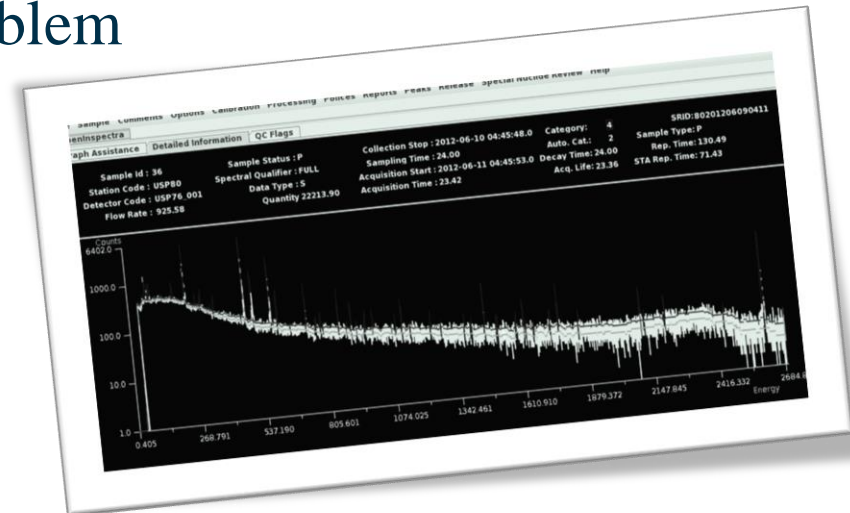


- Waveform data help identify the location of any event and qualify it as either natural or potentially man-made.
- However, they cannot reliably answer the question as to whether a man-made event, such as an explosion, was nuclear or not. The only reliable way to answer this question is to trace and **analyse** the radioactive remains of a potential nuclear explosion.
- Some remains provide the ultimate proof for the nuclear nature of an event
- Radionuclide monitoring data from the 80 radionuclide monitoring stations worldwide are expected to shed light on this key question.
- Data on radionuclide observations are sent to the International Data Centre (IDC), where they undergo an **analysis process**.
- After the **automatic analysis** process, analysts refine the results during interactive review.

- Only the **analysis of radionuclide** data can provide the ultimate proof to establish the nuclear nature of an explosion
- Each radionuclide particulate monitoring station sends one gamma ray spectrum per day showing which radionuclide were observed in a single sample and in what quantity.
- Each radionuclide Sample was examined and categorized in the corresponding group according to the nature of the radionuclide contained in them.

- In the spectrum analysis process, **doubts** about the existence of level 4 or 5 nuclides are made.
- In order to ensure that a **suspect nuclide** exists or not, this presentation addresses the problem of **association of unidentified peaks with suspect nuclides**.
- We assume that the corresponding energy is an amount of **sum of energies** provided by the **suspects nuclides**.

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- The **Subset Sum Problem** (SSP) is an important problem in computer science and combinatorial optimization.
- The challenge is to determine if there is some subset of numbers in an array that can sum up to some number s .
- SSP is to find subset of elements that are selected from a given set S whose sum adds up to a given number K , where we consider that the set S contains non-negative values.

Given :

$A = (a_1, a_2, \dots, a_n)$ and
a positive integer s , called the sum.

The question is then : Is there a subset A' of A with

$$SUM_{a' \text{ in } A'}(a') = s, \text{ or equivalent:}$$

Does there exist a vector

$$X = (x_1, x_2, \dots, x_n), x_i \text{ in } \{0, 1\}, \text{ with } AX = s?$$

If a solution is desired, the problem becomes a **functional problem**:

The functional problem of any vector A together with a sum s is denoted by (A, s) .

Input Data

- $A = (15, 22, 14, 26, 32, 9, 16, 8)$
- $s = 53$.

Solution

$(A, 53)$ is given by the vector $X = (1, 1, 0, 0, 0, 0, 1, 0)$, because

$$\begin{aligned} AX &= a_1 + a_2 + a_7 \\ &= 15 + 22 + 16 = 53. \end{aligned}$$

The corresponding subset is $A' = (15, 22, 16)$.

it's not the only solution

- Generally, there may exist several solutions to (A, s)
- Another solution for $(A, 53)$ is $X = (0, 1, 1, 0, 0, 1, 0, 1)$ with the subset $A' = (22, 14, 9, 8)$.

- The SSP is in the NP complexity class.
- The decision problem is NP-complete and the corresponding functional problem is NP-hard.
- No polynomial algorithm is known solving the general subset sum problem.
- The trivial possible solution vector for a given (A,s) is :
for all possible 0-1 vectors $\mathbf{X} = (x_1, \dots, x_n)$ the sum $s' = \mathbf{A}\mathbf{X}$ is computed.

But, this algorithm is computing the sum of all 2^n different \mathbf{X} vectors, and has an exponential running time of $O(2^n)$.

Meet-in-the-middle algorithm

- One of the more efficient algorithms;
- Recursive algorithm;
- At each iteration, this algorithm divides the original input vector A in two equal parts $A_1 = (a_1, \dots, a_t)$ and $A_2 = (a_{t+1}, \dots, a_n)$.
- All possible sums $s_1 = A_1 X_1$ are computed in a pre-computation step.

Meet-in-the-middle algorithm

- Input: a vector $A = (a_1, \dots, a_n)$ and a sum s .
- Output: a vector X with $AX = s$, provided a solution exists.

I- Divide $A = (a_1, \dots, a_n)$ into $A_1 = (a_1, \dots, a_t)$ and $A_2 = (a_{t+1}, \dots, a_n)$.

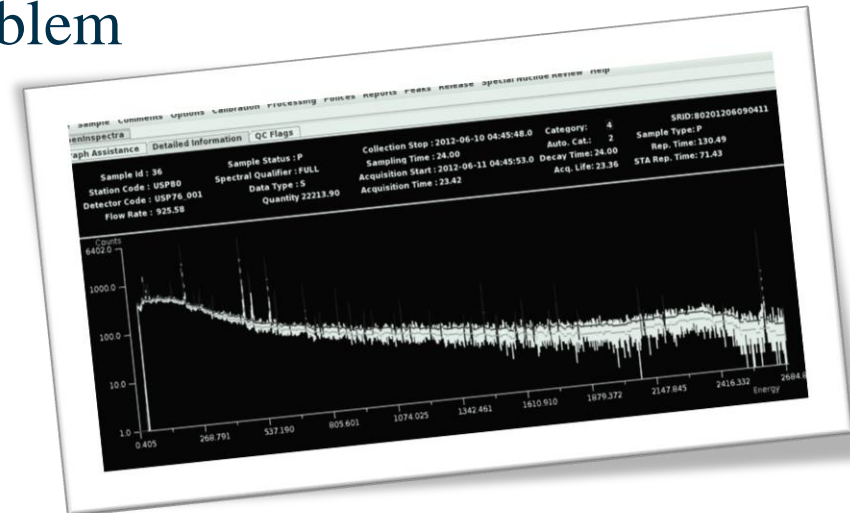
For every vector $X_1 = (x_1, \dots, x_t)$

- compute $s_1 = A_1 X_1$
- store s_1 together with the corresponding *x -vector* in a table T
- sort this table by the sum

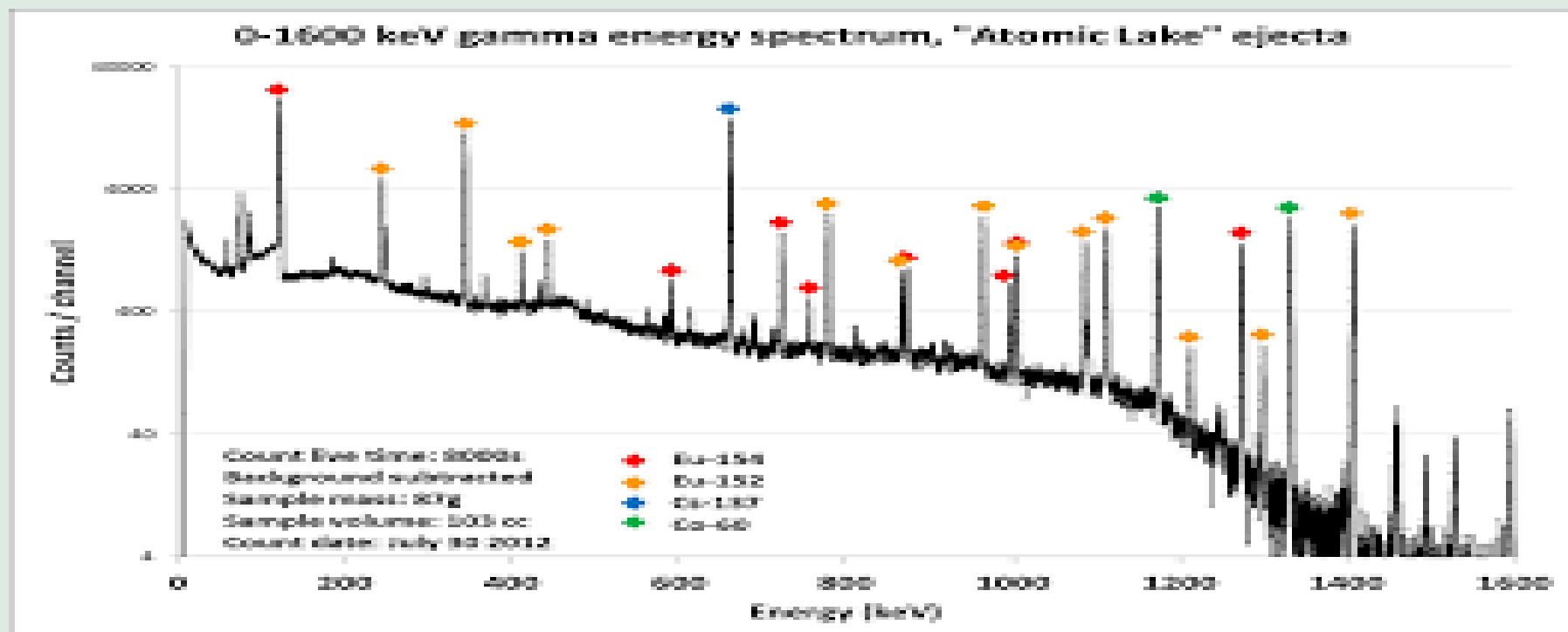
II- Now for all possible vectors $X_2 = (x_{t+1}, \dots, x_n)$

- compute $s_2 = A_2 X_2$
- get the difference $L = s - s_2$
- search L in T . If found, a solution vector is $X = X_1 || X_2$.

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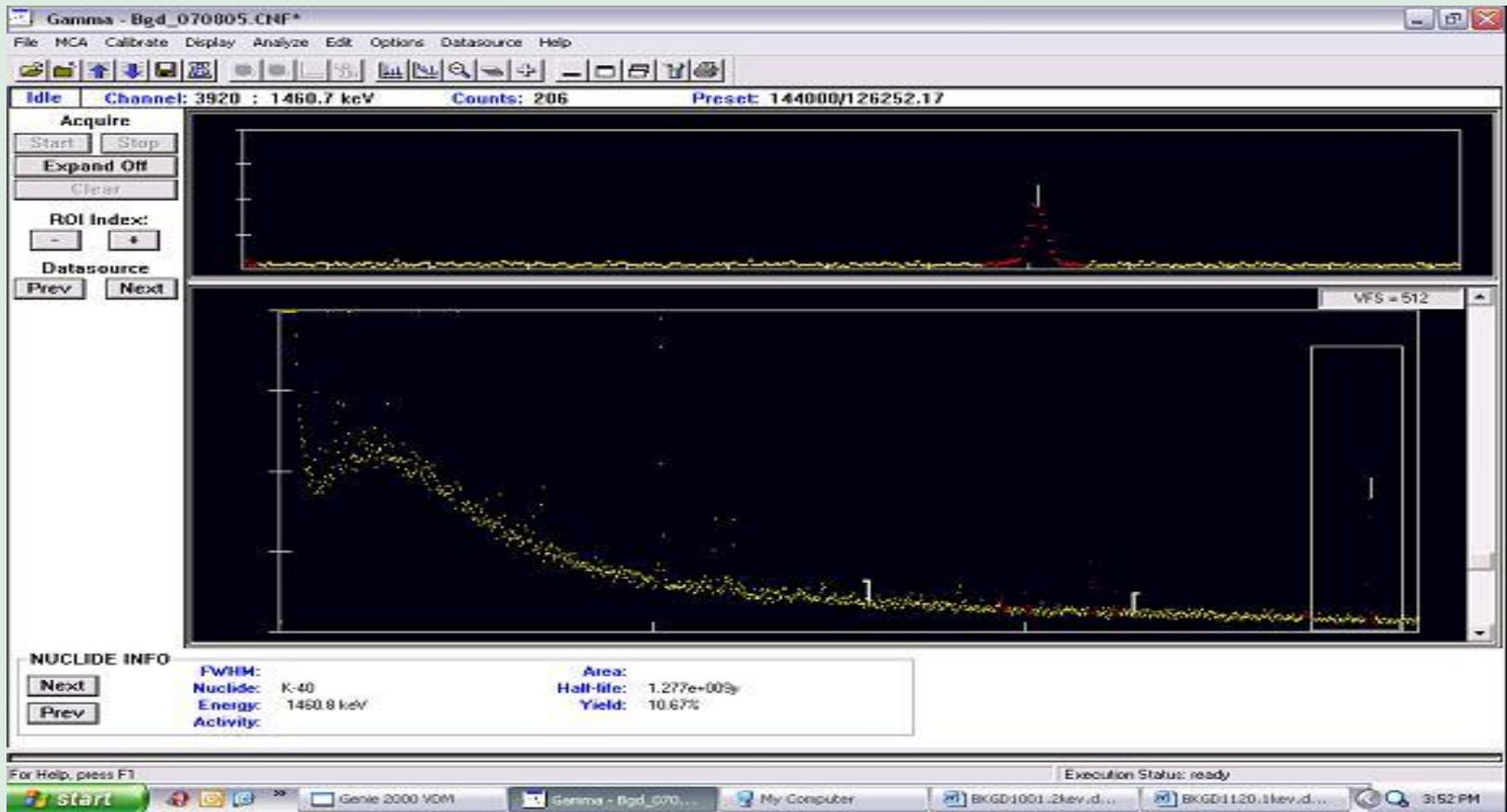


- Most radioactive sources produce gamma rays, which are of various energies and intensities. When these emissions are detected and analyzed with a spectroscopy system, a gamma-ray energy spectrum can be produced.



- Gamma spectrometry is one of the fundamental measuring techniques in nuclear technology for unambiguous, clear identification of radionuclide, even in mixtures of various isotopes.
- The experiment is intended to show the basics of the methodology of gamma spectrometry, the properties of most important gamma detectors and how to identify clearly radionuclides.
- Moreover, the absolute activity of a radionuclide could be determined by means of a gamma spectrometer if it is calibrated absolutely with regards to its efficiency.

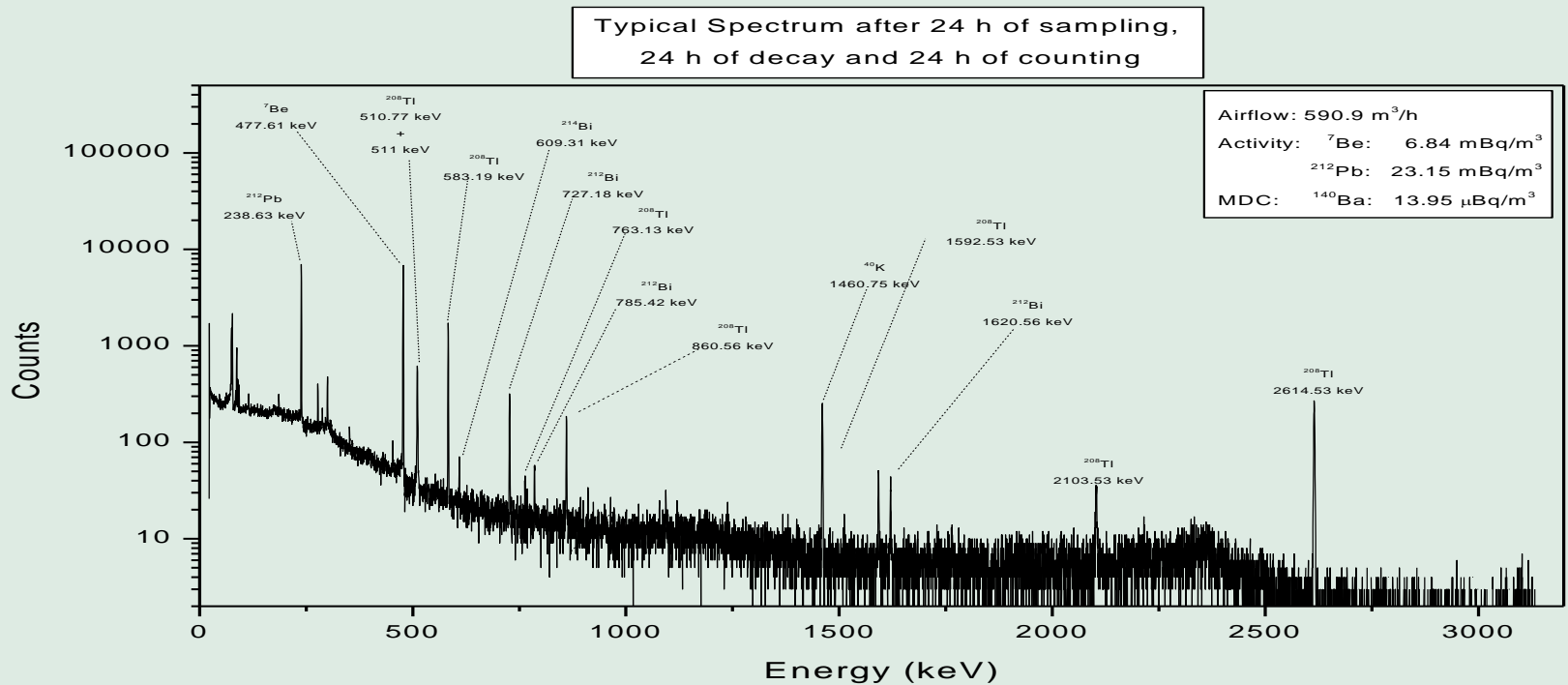
- For an IDC or NDCs Analyst, the Analysis of the identity of gamma-emitting radionuclides and measurement of their respective activity in a sample are the important tasks



Energy

Gamma emitters can be identified by their respective energies

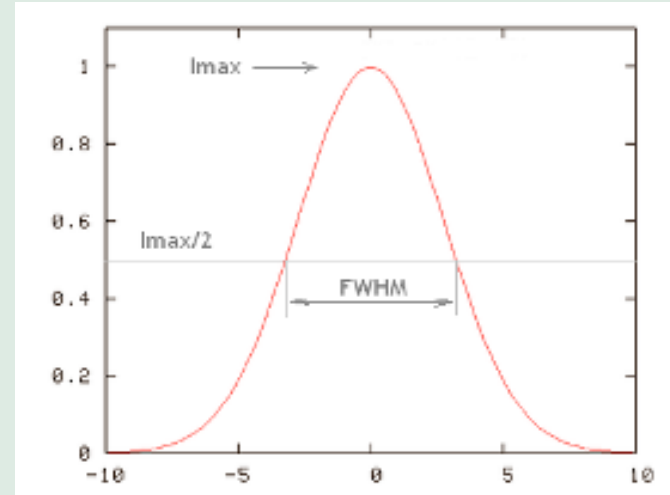
Important characteristic for detection – very low energy gammas are difficult to detect; **gamma emitters with similar energies are difficult to identify**



Detectors characteristics

Resolution

- ability to separate two gamma peaks that are close to each other in order to be able to separately measure and identify these peaks.
- usually measured with the full-width at half maximum (FWHM). This is the width of the gamma ray peak at half of the highest point on the peak distribution.
- A requirement for gamma detectors used in radionuclide stations is that the FWHM should be < 2.5 keV at 1332 keV (Co-60 peak)



Efficiency

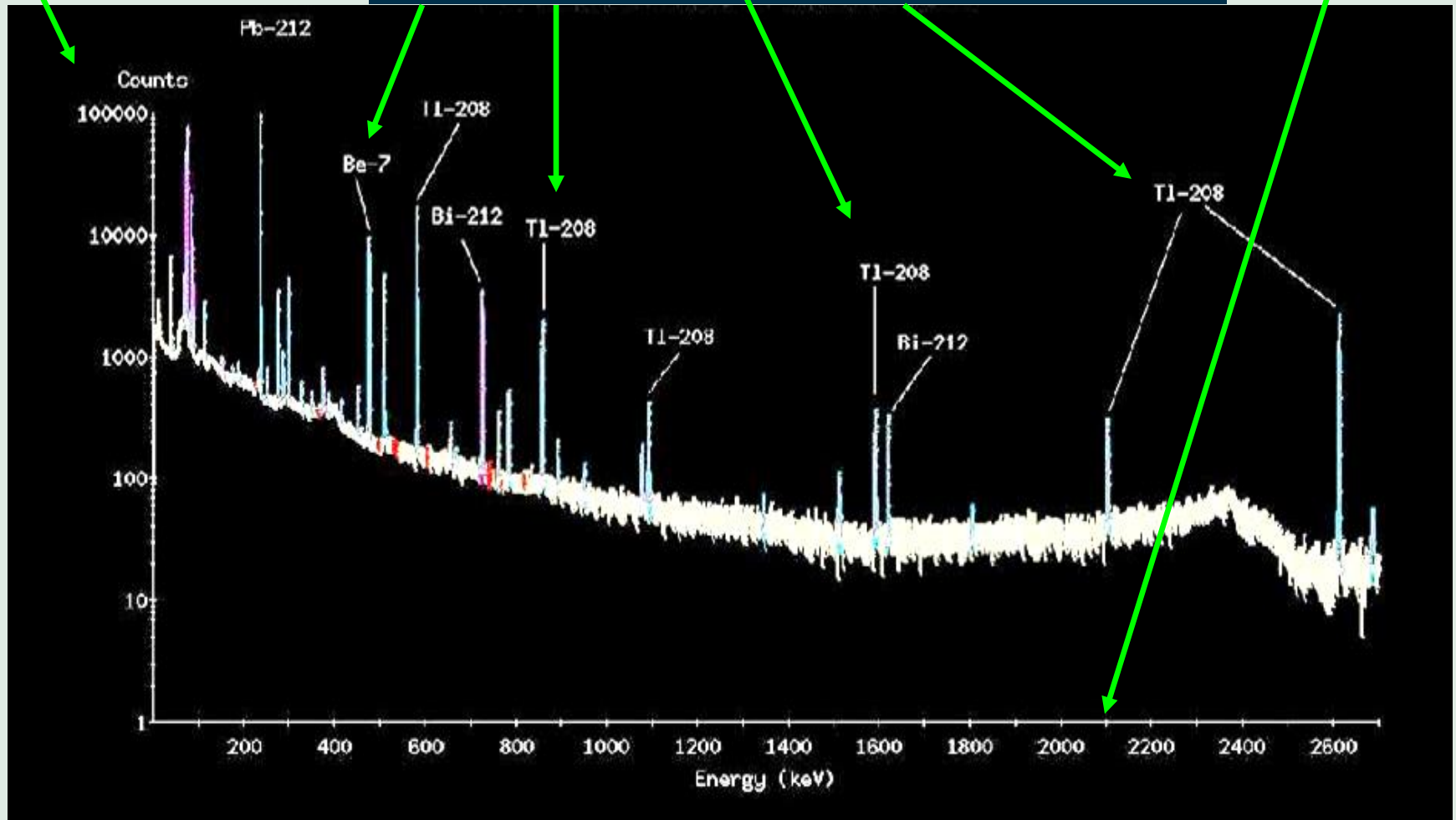
- Relative efficiency values are often used for germanium detectors, and compare the efficiency of the detector at 1332 MeV to that of a 3 in \times 3 in NaI detector (another gamma detector). This type of detector was popular and well characterized before the introduction of the germanium detectors.
- Relative efficiency of detectors used at radionuclide stations should be $\geq 40\%$. The higher the efficiency, the better the detection sensitivity.

Example of station sample spectra

Number of γ -photons collected in the detector

What energy do they have?

What radionuclides and how much are in the sample?



Software for interactive review : OpenSpectra

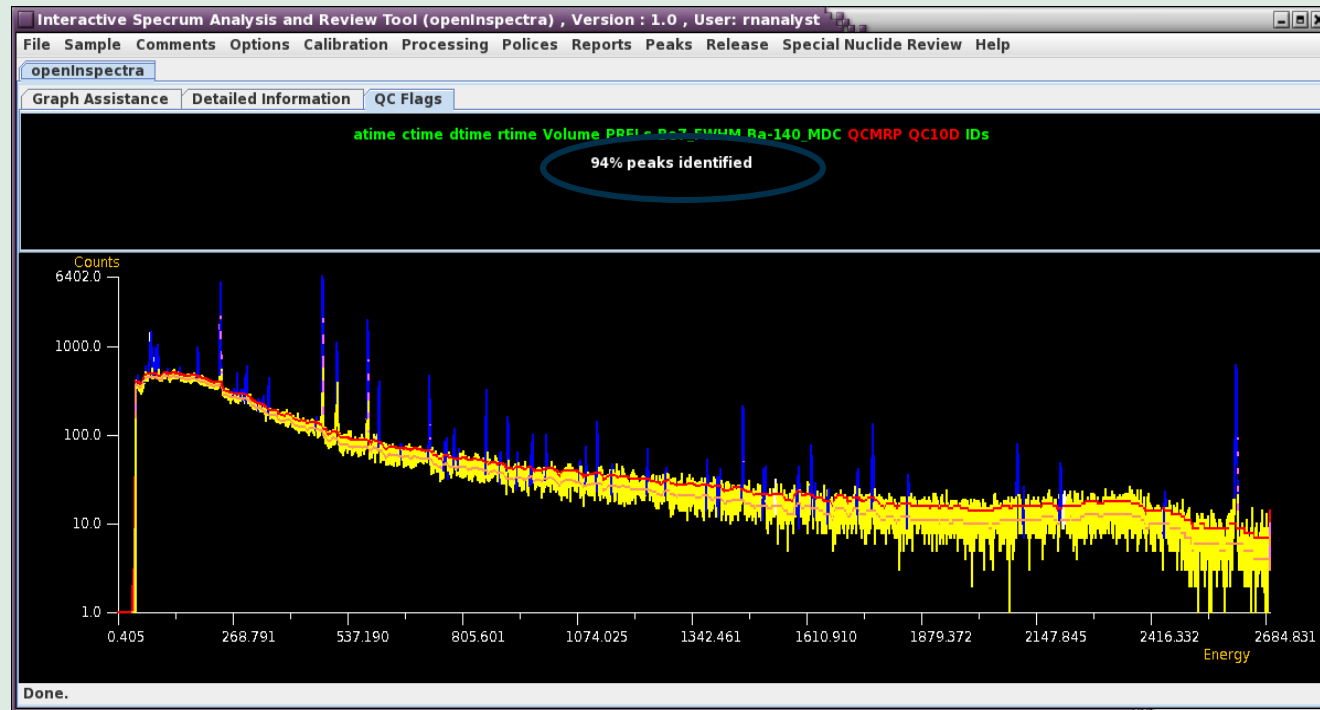
- A java-based license-free application for interactive review of automatic processing results which covers both particulates stations and Noble gas systems.

Sample metrics:

- Collection time
- Decay time
- Acquisition time
- Reporting time
- Be-7 FWHM
- Ba-140 MDC
- MRP QC
- QC 10 days
- %Identified peaks

Color coding:

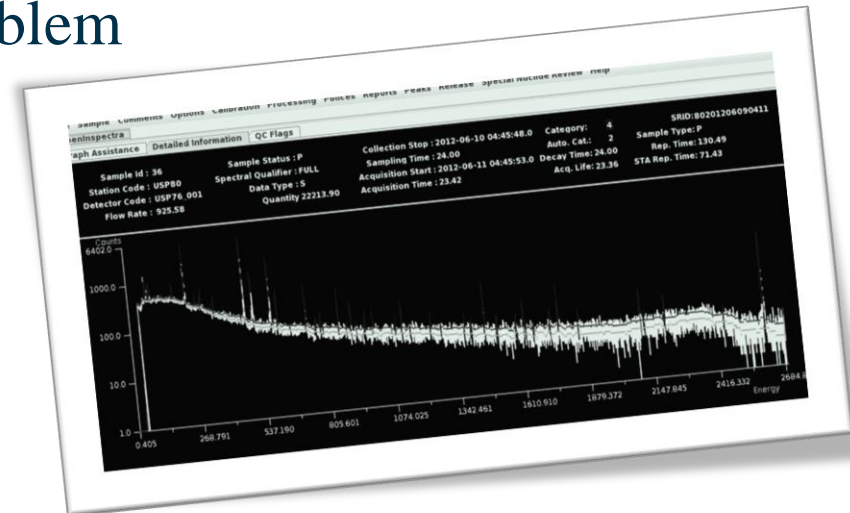
- GREEN: *Pass*
- RED: *Fail*



Software for interactive review

- Some of peaks (value of energy) are sometimes not identified;
- One of main analyst tasks is to affect the correct nuclide to the corresponding value of energy. This task allows the precise identification and quantification of the elements;

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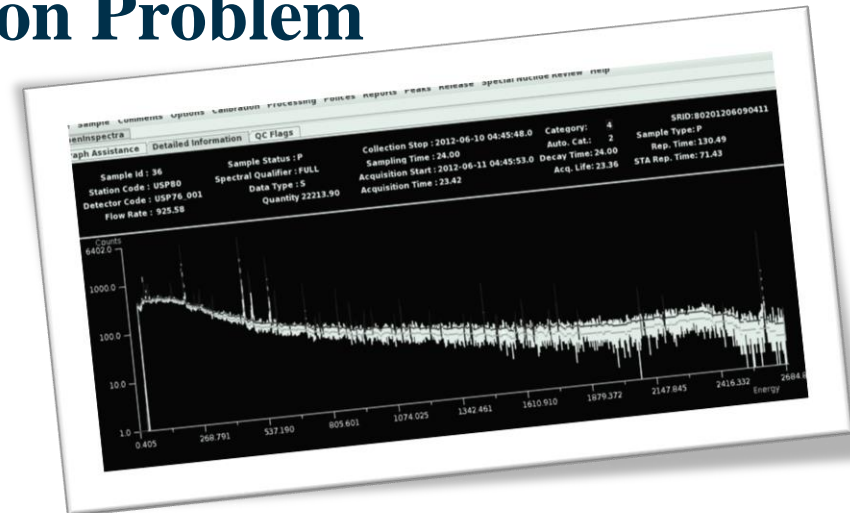


- One of main analyst tasks is to affect the correct nuclide to the corresponding value of energy. This task allows the precise identification and quantification of the elements;
- Some of peaks which corresponding to a given value of energy are sometimes not identified;
- The non-identification is due to the fact that the corresponding energy does not correspond to any classified nuclide;
- In order to identify such a peak and associates it with one or more radionuclide, we apply a formulation of a subset sum problem.

- In fact, there are some peaks that are already associated to the corresponding radionuclide (automatic identification peak).
- These radionuclides along with **suspect radionuclides** are candidates to be the source of energy corresponding to the unidentified peak
- The problem can be expressed by the following :

From already detected radionuclides and the set of suspect radionuclides, what are the radionuclides whose energy accumulation corresponds to the energy of the unidentified peak.

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- This problem can be formulated as a **functional problem** (A,s) of a **subset sum problem** as follows:

Input :

A : the vector which contain energy value of all existing radionuclides, together with energy value of suspect radionuclides

s : The energy of the unidentified peak (the peak which is not yet associated with a radionuclides)

Output :

The set of energy value selected (radionuclide detected). Then, the peak become identified

- Let $A = (a_1, \dots, a_n)$ a set of energy value of all existing radionuclides, together with energy value of suspect radionuclides
- Let $X = (X_1, \dots, X_n)$ a set of boolean decision variable where
 - $X_i = 1$ if the corresponding energy selected
 - $X_i = 0$ otherwise
- Given s the energy of the unidentified peak

Identification of the peak consist on selecting a subset of X whose total corresponding energies is closest to, without exceeding, the value s

- Integer linear program ILP formulation

$$\text{Maximize } z = \sum a_i X_i$$

Subject to

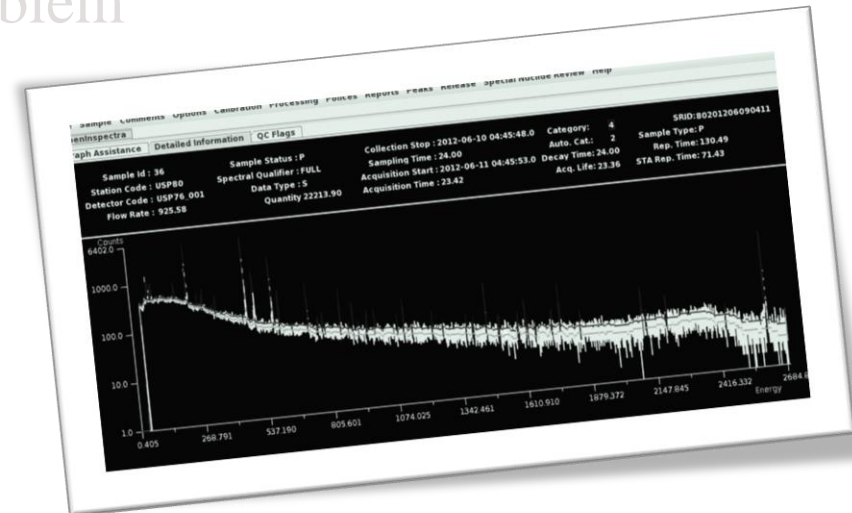
$$\sum a_i X_i \leq s$$

$$X_i = 0 \text{ or } 1$$

Many approach resolution to the SSP problem

- **Exact Algorithms** *Faaland (1973); Ahrens and Finke(1975); Martello and Toth (1984)*
 - Dynamic programming,
 - Branch and bound method
- **Approximate Algorithms**
 - Greedy algorithms,
 - Polynomial time approximation schemes
 - fully polynomial time approximation schemes
 - Probabilistic analysis
- **Hybrid Algorithms**

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- SSP formulation for the problem of assignment of radionuclides to any peak without accordance energy-radionuclide;
- Our idea allows the analyst to reduce the number of unidentified peaks
- The SSP can be solved in polynomial or pseudo polynomial time for small instances
- The SSP formulation is very effective for testing the existence of such radionuclide which have several levels of energy

Thank you for your attention

