Development of Monte Carlo code for Coincidence Prompt Gamma-ray Neutron Activation Analysis

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Agenda

- Overview (PGNAA and CPGNAA)
- Monte Carlo code CEARCPG
- Benchmark Experiments
- Conclusion

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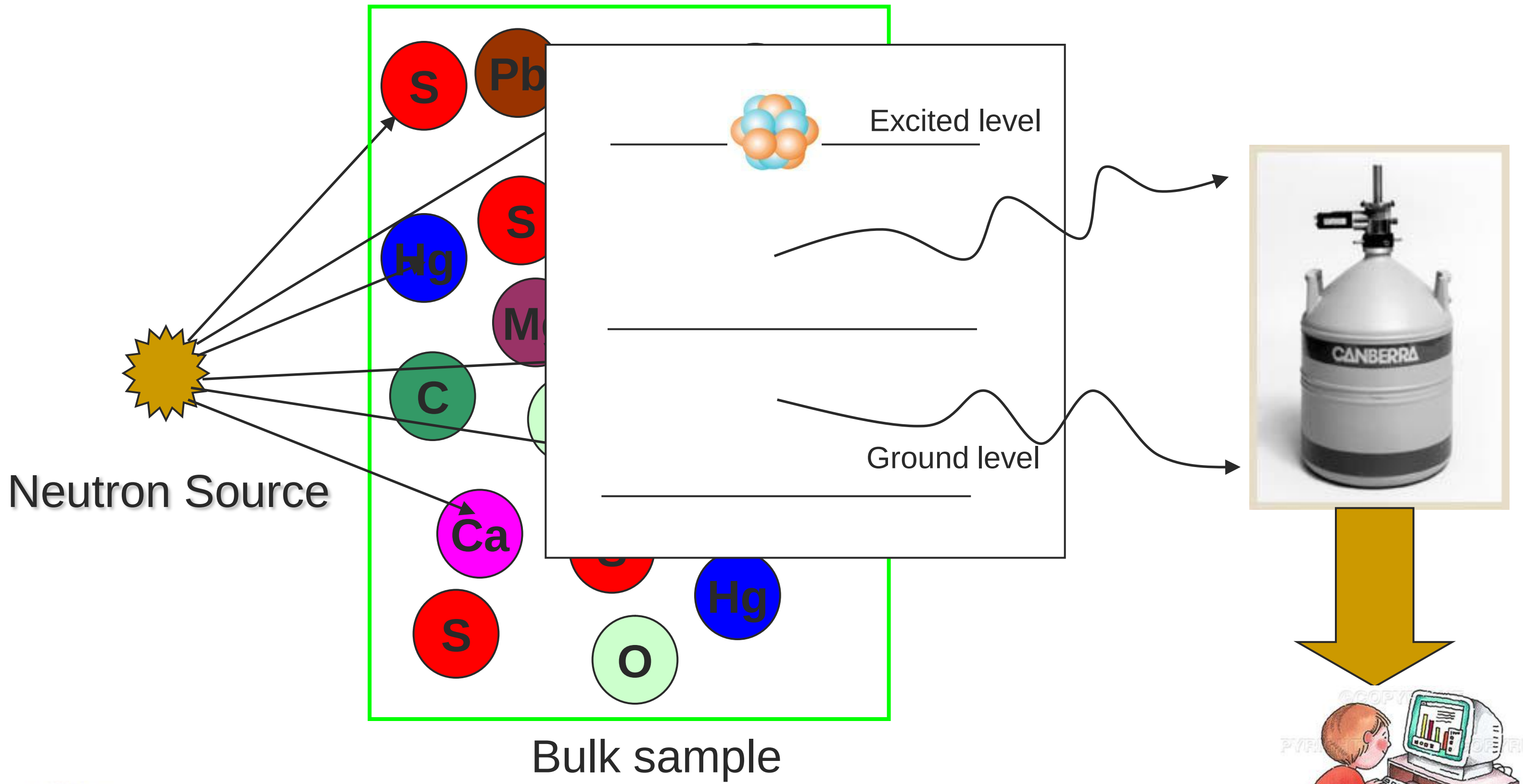
Overview-PGNAA



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Overview-PGNAA

- Advantages:
  - Nondestructive
  - Simultaneous
  - In Situ
  - Quantitative
  - sensitive to the entire periodic table.
  - shape of the sample are relatively unimportant.

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Overview-PGNAA

- Disadvantages
  - PGNAA has an inherently large background
    - Interference from the neutron excitation source.
    - Natural background
    - Structure materials
    - Detector activation (NaI)
    - Summing and pulse pile-up effect

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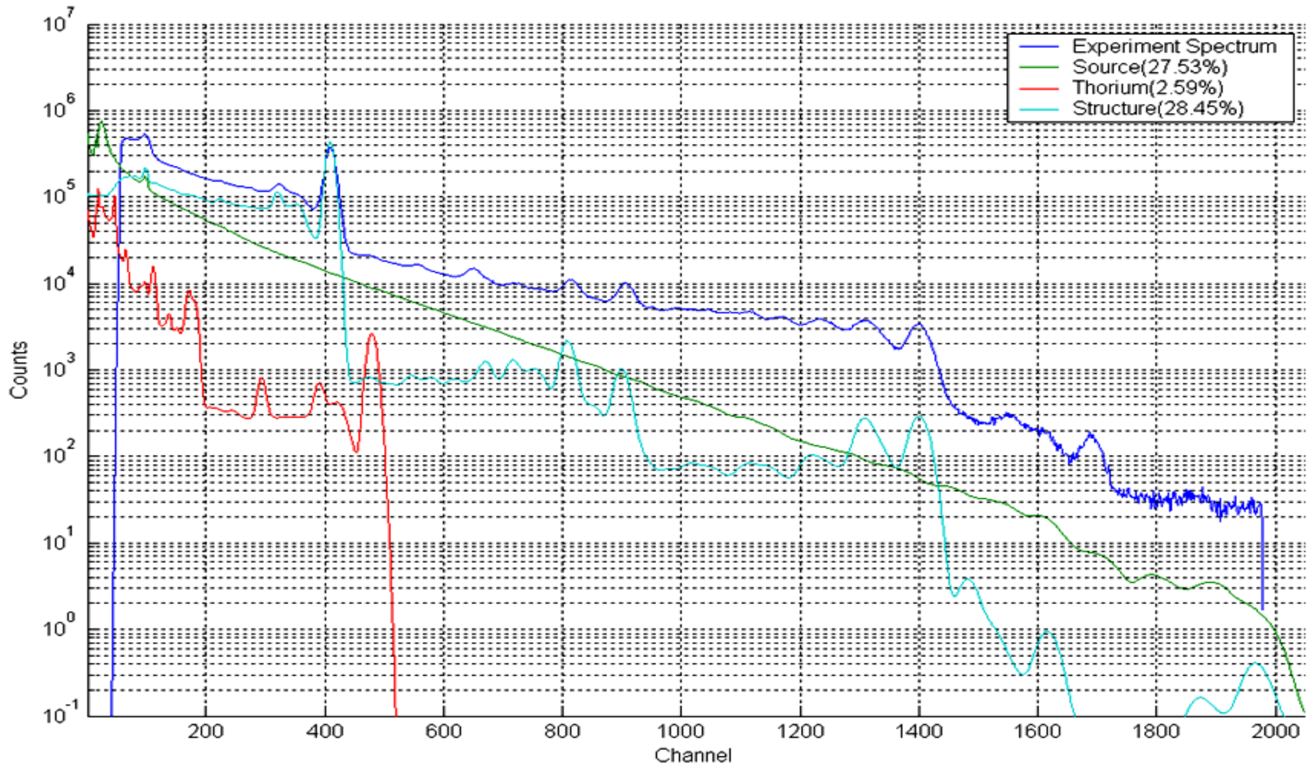
Overview-PGNAA



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Overview-PGNAA

- Improvement: introduce gamma – gamma coincidence technique (CEAR and BNC, Budapest Neutron Center)
- Advantages of gamma – gamma coincidence technique
  - Increase the signal – to – noise ratio
  - Reduce the interference of background
  - Eliminate the hydrogen prompt gamma-ray peak

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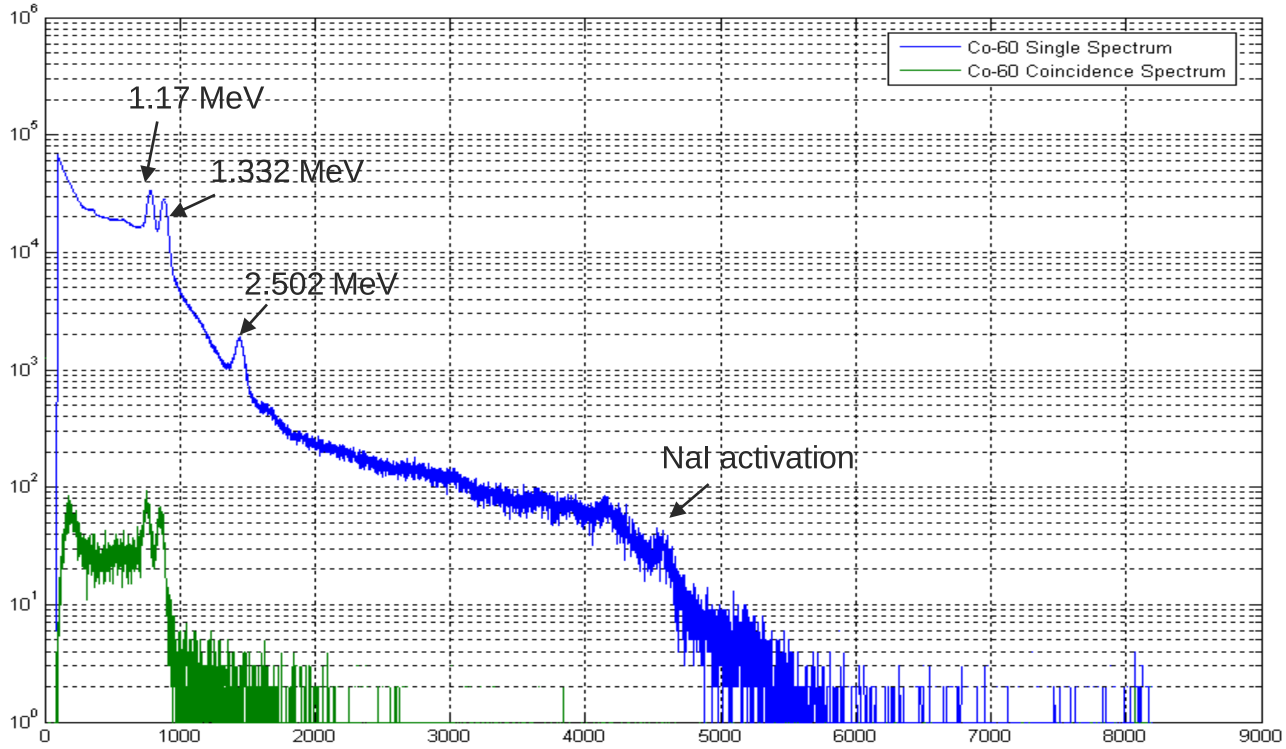
Overview-Coincidence measurement



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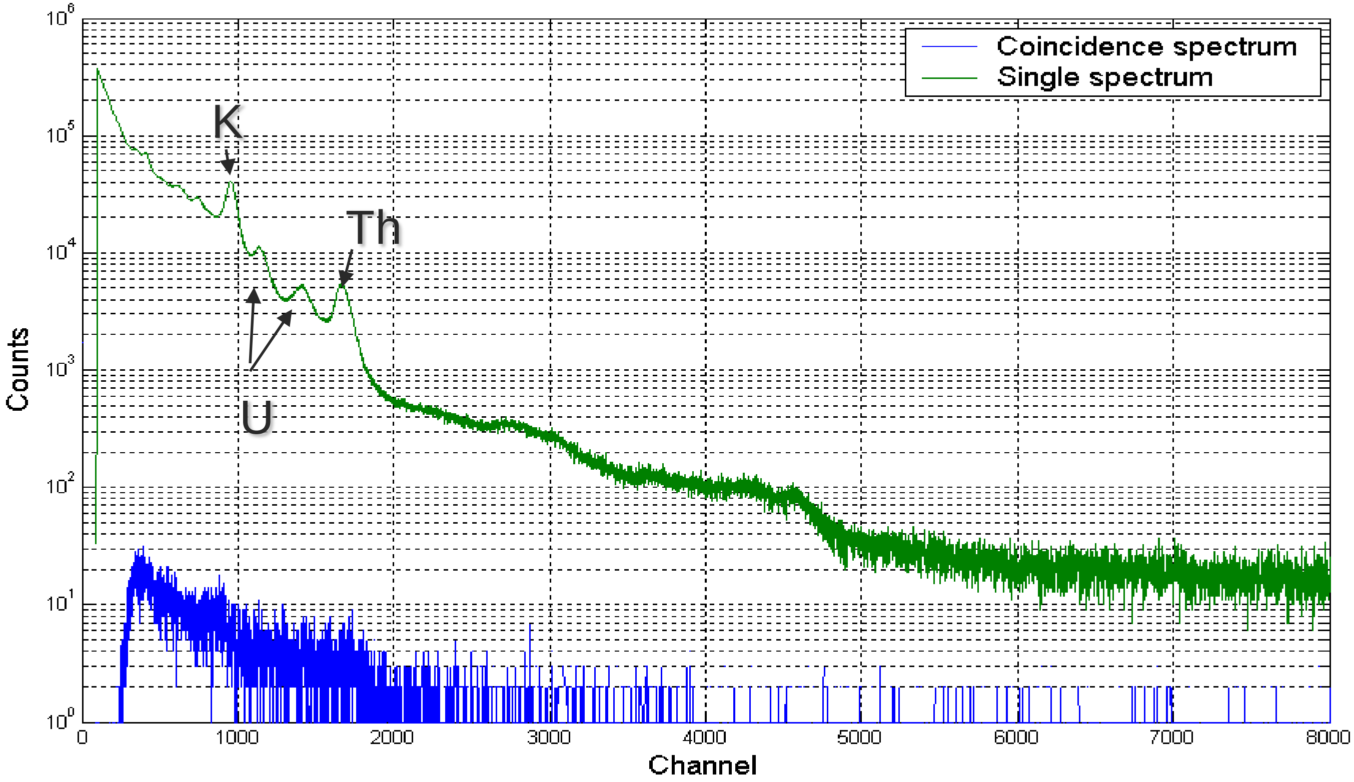
Overview-Coincidence measurement



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Overview-MC work

- CEARPGA I, the first specific Monte Carlo code publicly reported to implement MCLLS algorithm for PGNAA analyzer
  - Big weight problem
  - Detector response function
  - Library spectrum (natural background, NaI activation)
- CEARPGA II
  - Interpolation
  - NaI activation spectra

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Physics – neutron reaction

- Neutron capture reaction
- Neutron elastic scattering reaction
- Neutron inelastic scattering reaction
- Thermal neutron scattering
    - Free gas model

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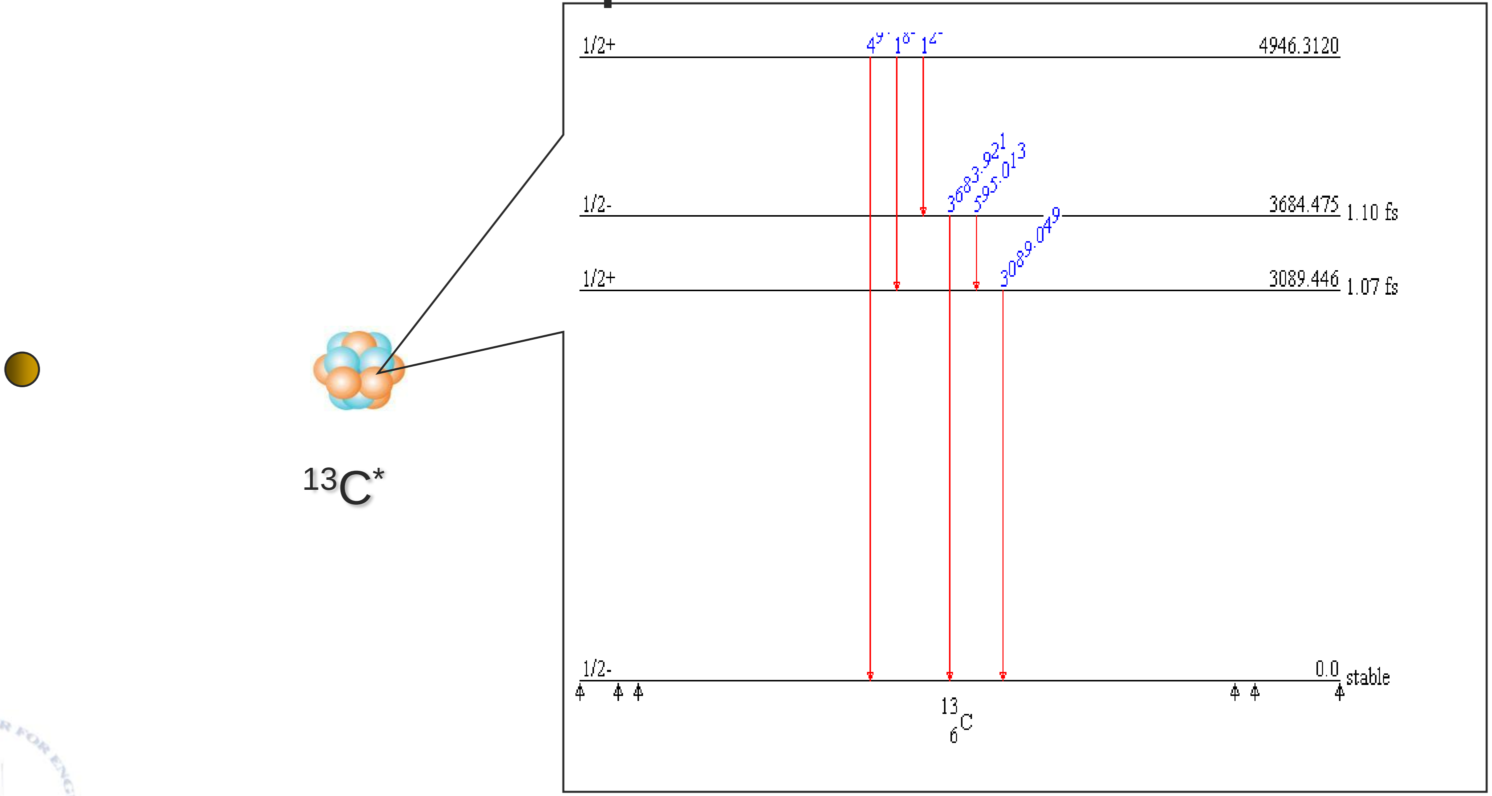
Physics – neutron reaction

- Neutron Capture reaction



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Physics – neutron reaction

```
13C     *12C(N,G) E=TH                    1982MU14                    91NP     200006
13  6 I      4          6          0          0          0                    0
      H TYP=FUL$AUT=F. AJZENBERG-SELOVE, J.H. KELLEY AND C.D. NESARAJA$
    2 H CIT=NP A523, 1 (1991)$CUT=1-Jul-1990$
     c  Target J|p=0+.
     c  1982Mu14: measured E|g and I|g, deduced S(n).
     c  Evaluated S(n)=4946.31 keV (1995Au04).
     cL E          From E|g using least-squares fit to data.
     cL J,T        From 1996FiZY, except as noted.
     cG E          From 1996FiZY, except as noted.
     cG E(A)       From level energy differences.
     cG RI         Intensities per 100 neutron captures from 1982Mu14.
      N 1
     PN
   1  L 0.0        1/2-                 STABLE
   2  L 3089.446   161/2+               1.07 FS   10
   1  G 3089.049   20 0.43   2
   3  L 3684.475   171/2-               1.10 FS   9
   2  G  595.013   11 0.24   1
   1  G 3683.921   2332.14   64
S  4  L 4946.3120  231/2+
S  4 cL J          from s-wave neu
   3  G 1261.764   1232.36   44
   2  G 1856.716   12 0.16   1
   1  G 4945.301   3 67.47   92
```

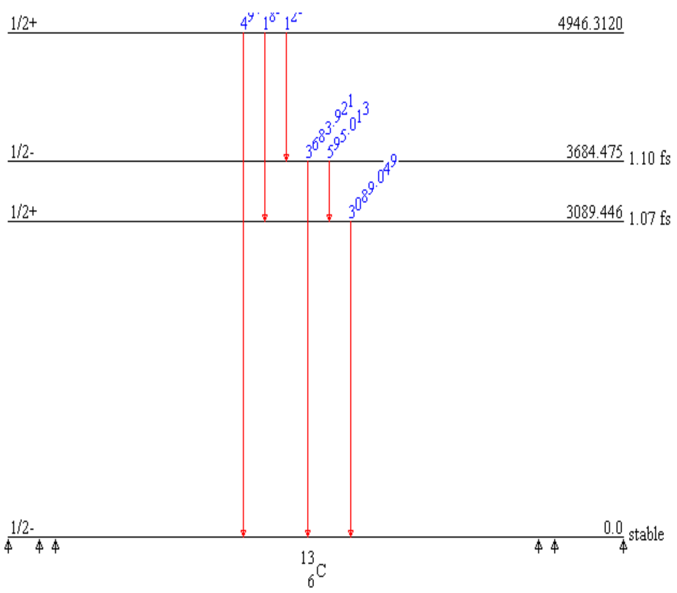
Level energy

Level life time

Relative intensity

Energy of Gamma ray generated from level 3

The ending level



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Physics – photon reaction

- Photon Pair-production reaction
  - Electron and positron deposit energy locally
  - Annihilation photons are tracked independently
- Photoelectron reaction
  - Photon-Electron deposit energy locally
- Compton scattering reaction

$$E' = \frac{E}{1 + \frac{E(1-\cos\theta)}{m_0 c^2}}$$

  - Angular distribution: *Klein-Nishina formula*

$$\frac{d\sigma}{d\Omega} = Z r_0^2 \left(\frac{1}{1+\alpha(1-\cos\theta)}\right)^2 \left(\frac{1+\cos^2\theta}{2}\right)\left(1 + \frac{\alpha^2(1-\cos\theta)^2}{(1+\cos^2\theta)[1+\alpha(1-\cos\theta)]}\right)$$

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CEARCPG-introduction

- Why we need to develop MC code
  - No existence MC code for coincidence PGNAA application
  - Specific MC code can be used to optimize the coincidence PGNAA application design. It also can be used to predict and check the experiment results.
  - It can be used to develop new algorithm for coincidence PGNAA analysis

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CEARCPG-introduction

- The first specific Monte Carlo Code that can be used for prompt gamma sampling and for prompt gamma coincidence spectra simulation.
- Coded in Fortran 95 on windows platform.
- Dynamic memory allocation
- Can be used to analyze 42 elements, 97 isotopes and easy to update.
- Neutron energy is from 10^{-11}MeV to 20 MeV. Gamma energy is from 1 keV to 20 MeV
- Most of CEARCPG cards take the same form as those used in MCNP.
- Modularized code. Easy to implement to other MC code
- General geometry package
- Detailed physics model
- Variance reduction techniques

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CEARCPG-introduction

- CEARCPG-Geometry
  - General geometry package treats an arbitrary 3-dimensional configuration of user-defined materials in geometric cell bounded by first or second-degree surface
  - Compatible with MCNP. Visual editor can be used to design and check the user-defined geometry.

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CEARCPG-introduction

CEARCPG-Variance reduction techniques

- Neutron
  - Stratified sampling
  - Russian roulette
  - Truncated Exponential pdf
  - Rejection method
  - Splitting
- Photon
  - Russian roulette
  - Energy cutoff
  - Truncated Exponential pdf
  - Rejection method

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CEARCPG-introduction

```
Created on: Monday, December 29, 2003 at 22:50
    1      1  -11.34      -1  2   -4  5   -6  7
    2      1  -11.34      5  -4   -2  40  7   -6  8
        ......
   44      6  -1.06       -41  35  -27  30
   45      6  -1.06       -42  33  -27  29

    1        pz        23.5
    2        pz          23
    3        pz        13.3
        ......
   41       c/z         14           0        8.3
   42       c/z        -14           0        8.3

m1     82000              -1.0
        ......
m8     13027              -1
imp   1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
      1 1 1 1 1 1 1 1 0 0 0 1 1 1
sdef    cf x=0.0  y=0.0  z=18  icel=3
nps     300000
number_detector 2
detector   -14.0 0 -25.8  7.62  15.24  16
           12.73 0 -24.53 7.62  15.24  21
sample   12
wcut 1d-6 1d-7 1d-10 1d-11 0.02
spect    2048 512 0 0  0.0055575  18000  0.0055575 0.02223
detcoin 1 ( 16 : 21 )
```


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CEARCPG-introduction

	CEARCPG	MCNP
Nuclear data	ENDF/B-VI ENSDF EPDL	ENDF/B-VI with NJOY format EPDL
Neutron interaction	Neutron capture reaction	Same
	Neutron elastic scattering reaction (Free gas thermal Treatment)	Same
	Neutron inelastic scattering reaction (n, n'γ)	All inelastic scattering reaction, such as (n.n') (n,2n) etc.
Generation of neutron-induced photons	Sampling from isotope scheme	The number is function of neutron weight, photon limit weigh, photon production cross section, etc. Expanded photon production method &30X20 photon production method
Photon interaction	Simple Physics Treatment	Simple Physics Treatment & Detailed Physics Treatment
Variance reduction technique	Stratified sampling	General

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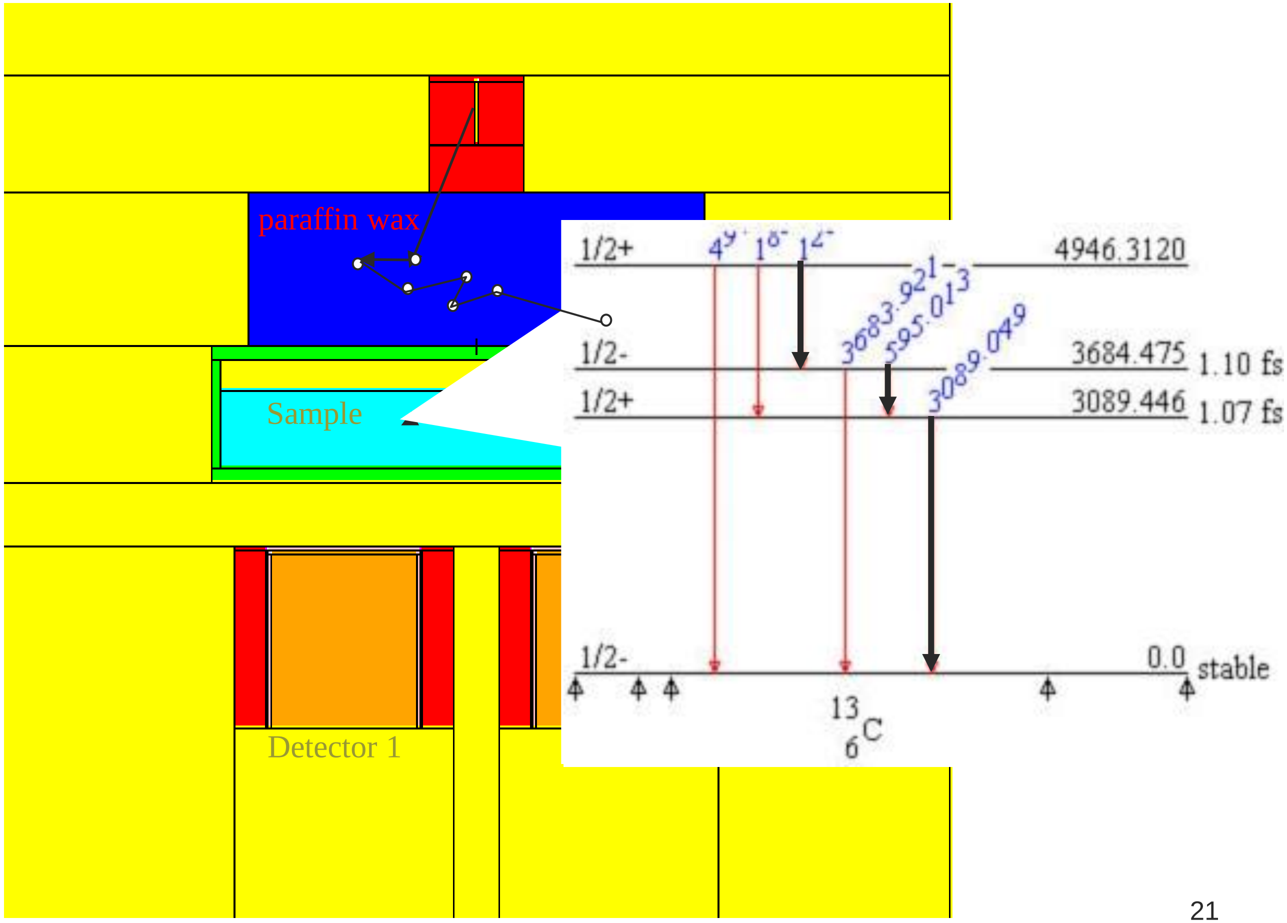
CEARCPG-introduction



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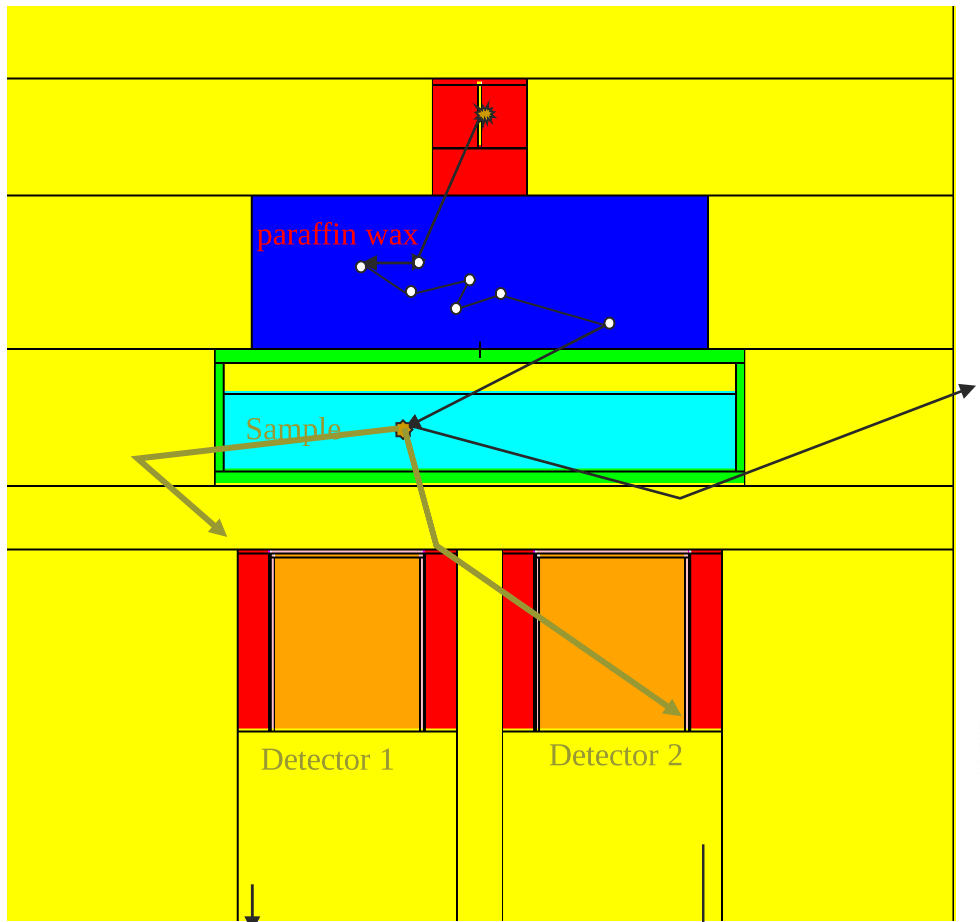
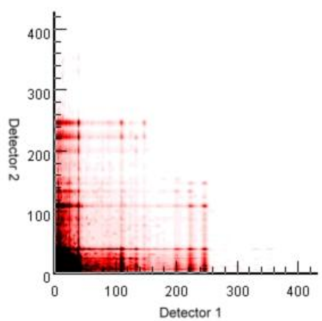
CEARCPG-introduction





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Benchmark Experiments

- ETI prototype. Coal sample Simulation and fitting
- Pure sulfur sample. Experiment, simulation and fitting
- Pure mercury sample. Experiment, simulation and fitting

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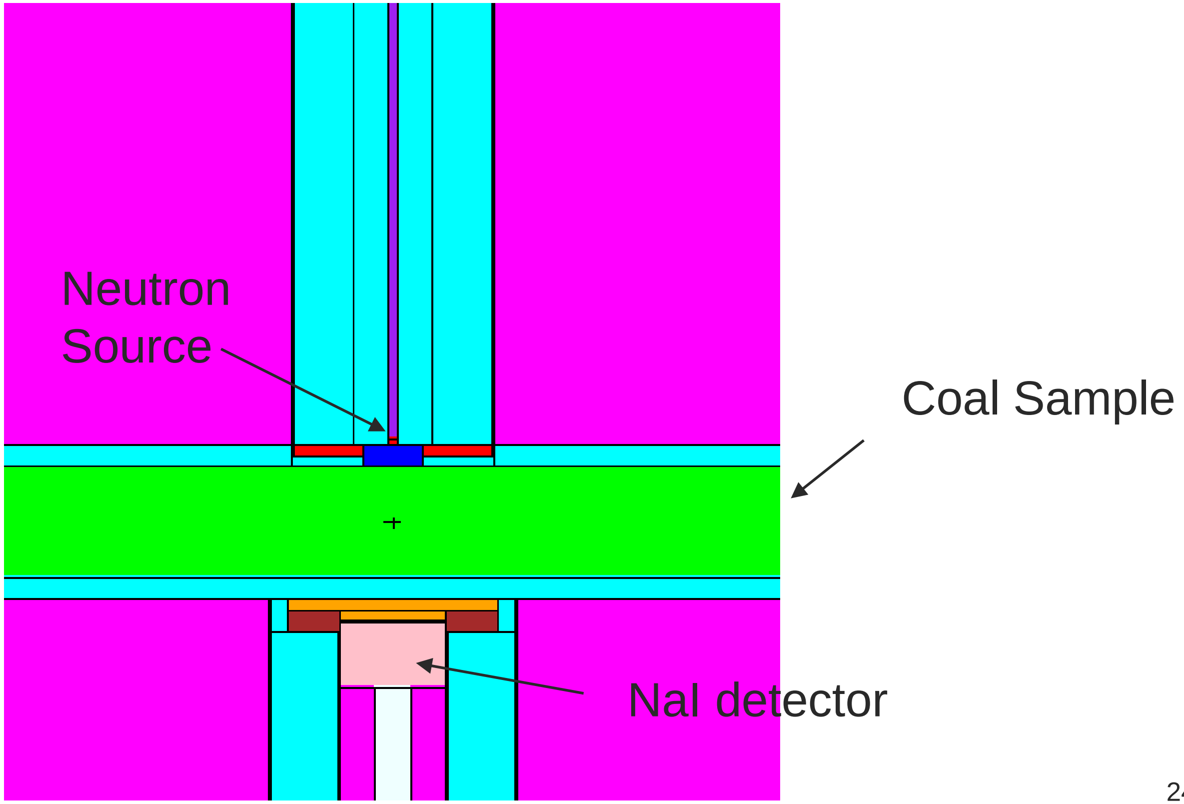
Benchmark Experiments

- ETI prototype



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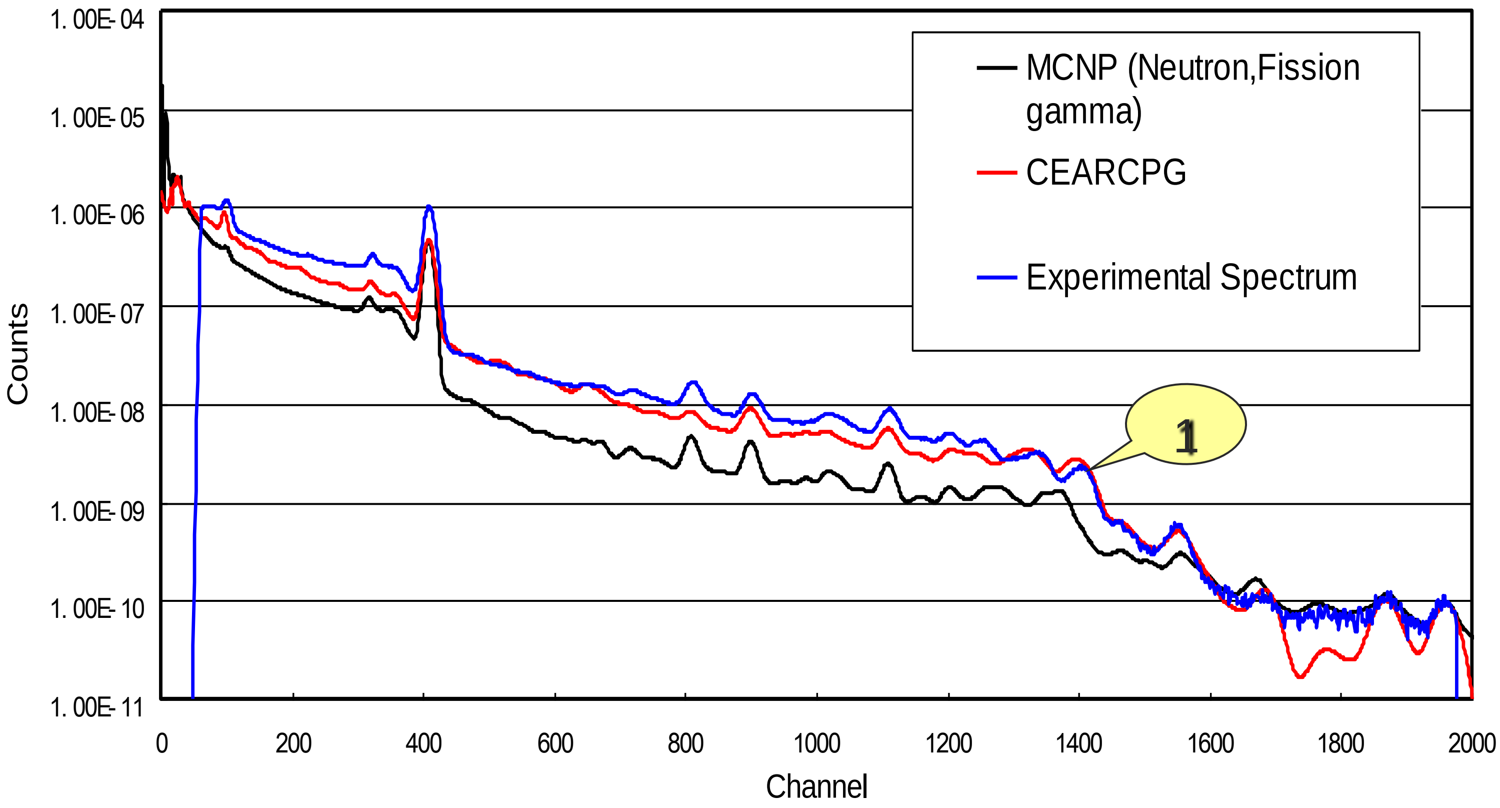
Benchmark Experiments



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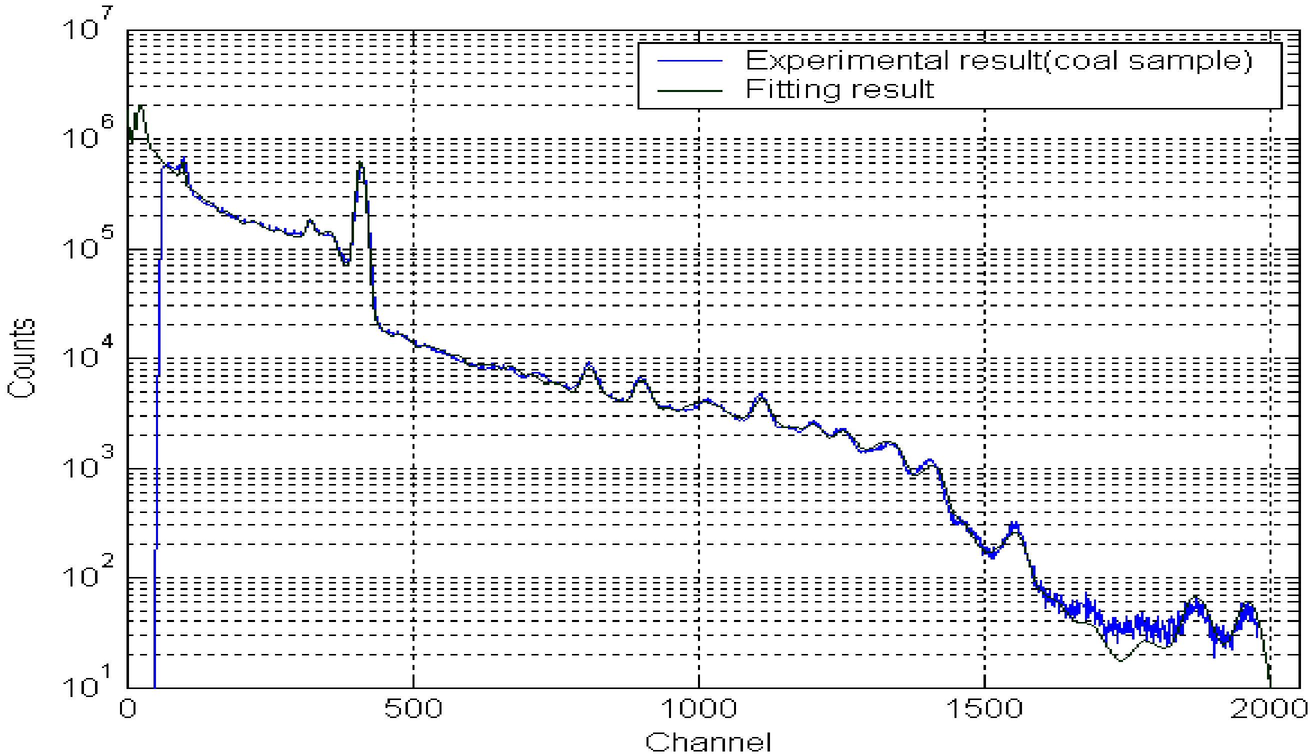
Benchmark Experiments



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Benchmark Experiments

Sample number	True weight fraction of sulfur	Calculated weight fraction	Relative error (%)
1	0.57	0.59	3.51
2	0.68	0.745	9.56
3	0.36	0.492	36.67
4	0.78	0.707	9.36
5	0.61	0.543	10.98
6	1.19	1.06	10.92

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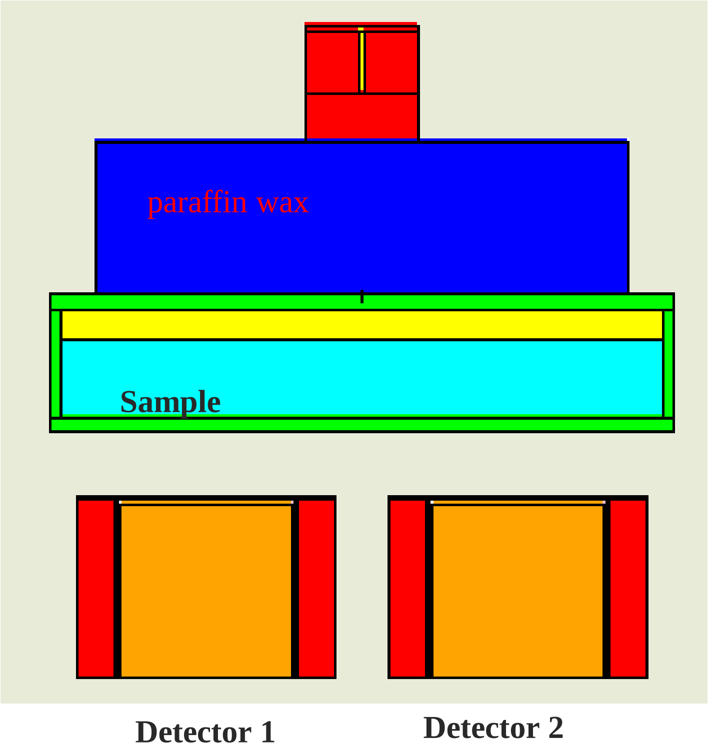
Benchmark Experiments

- Experiment 2 pure sulfur sample



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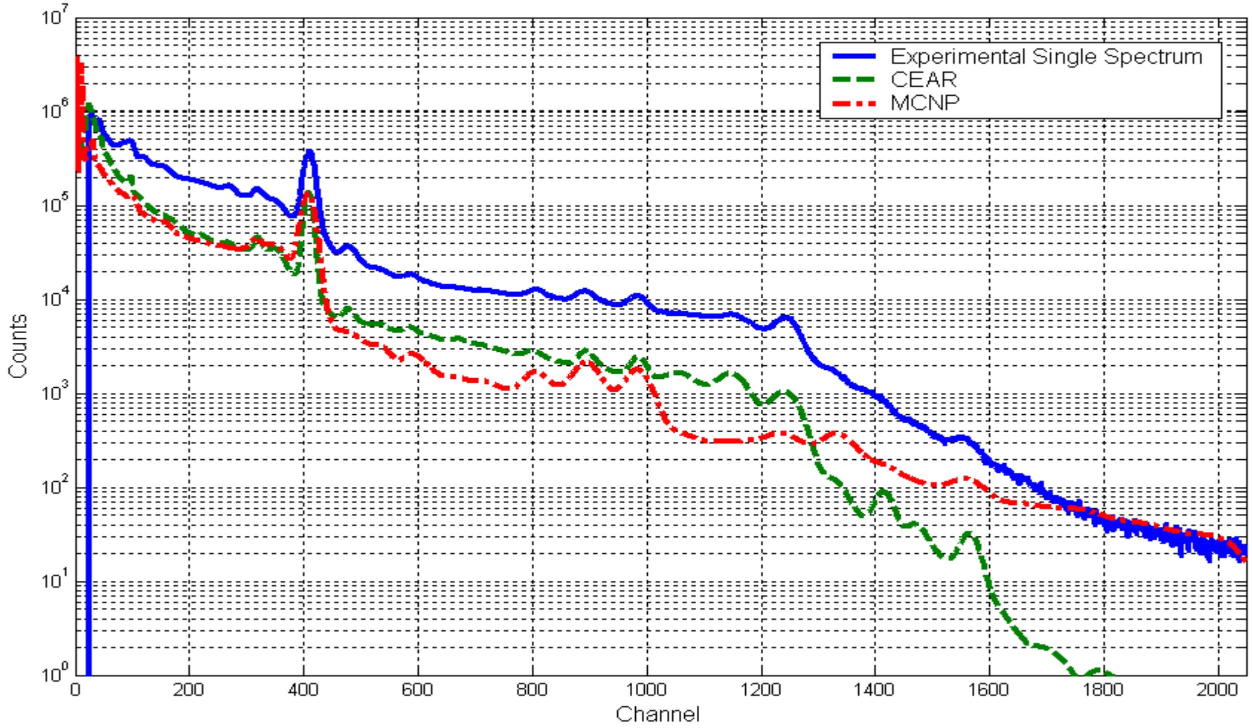
Benchmark Experiments



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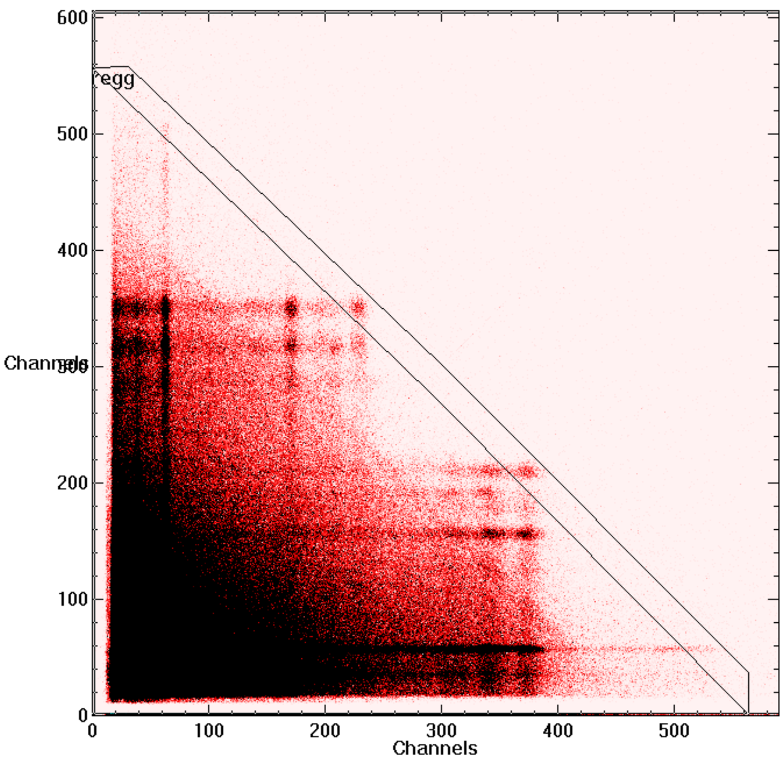
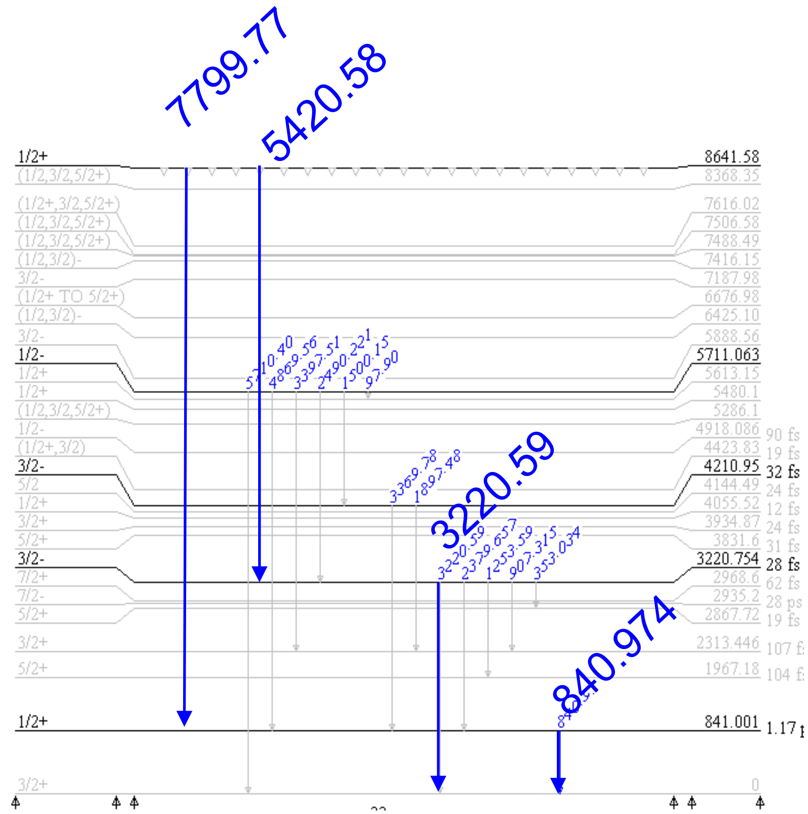
Benchmark Experiments





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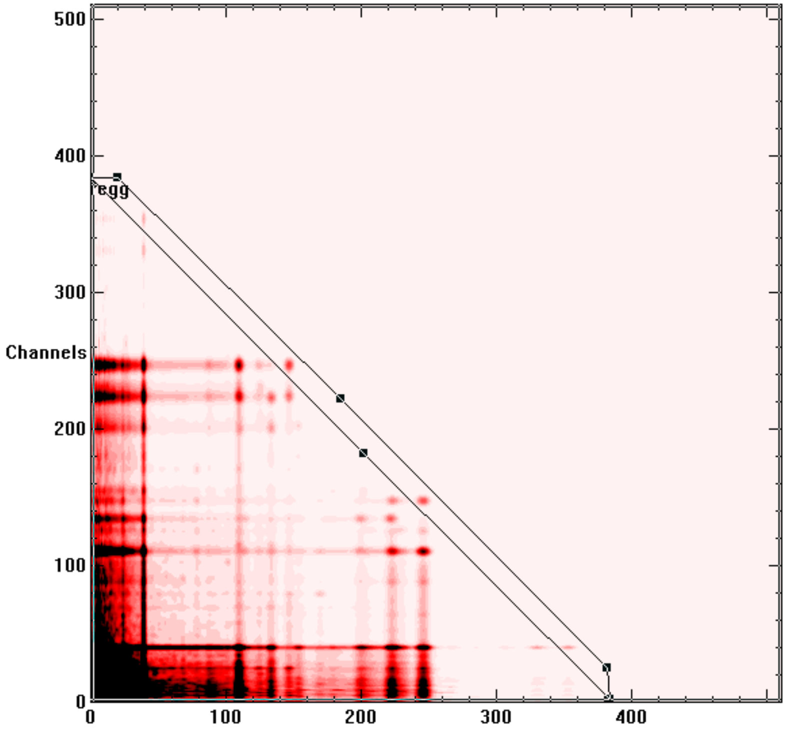
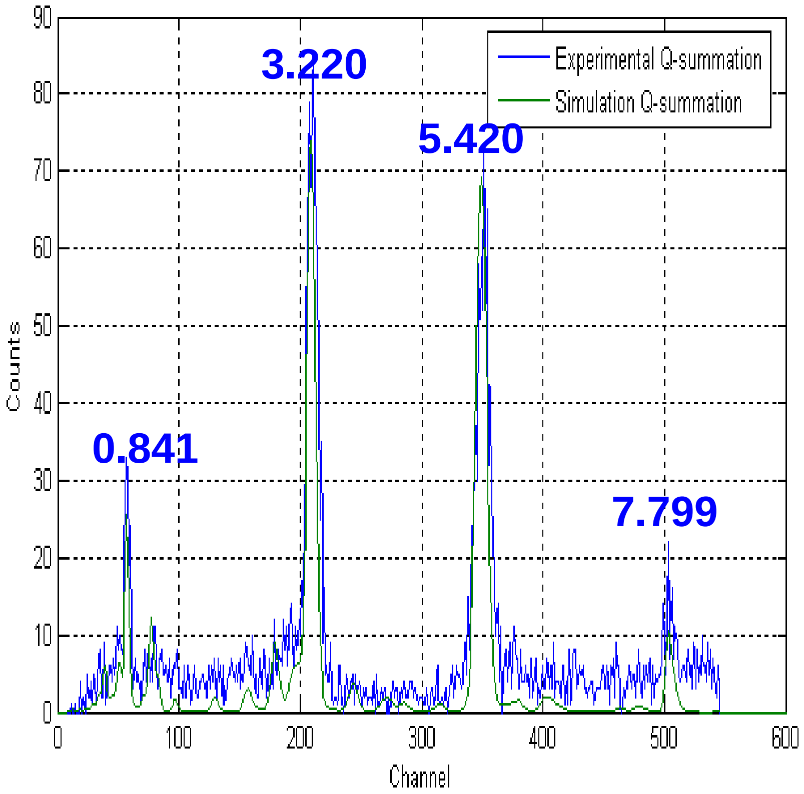
Benchmark Experiments





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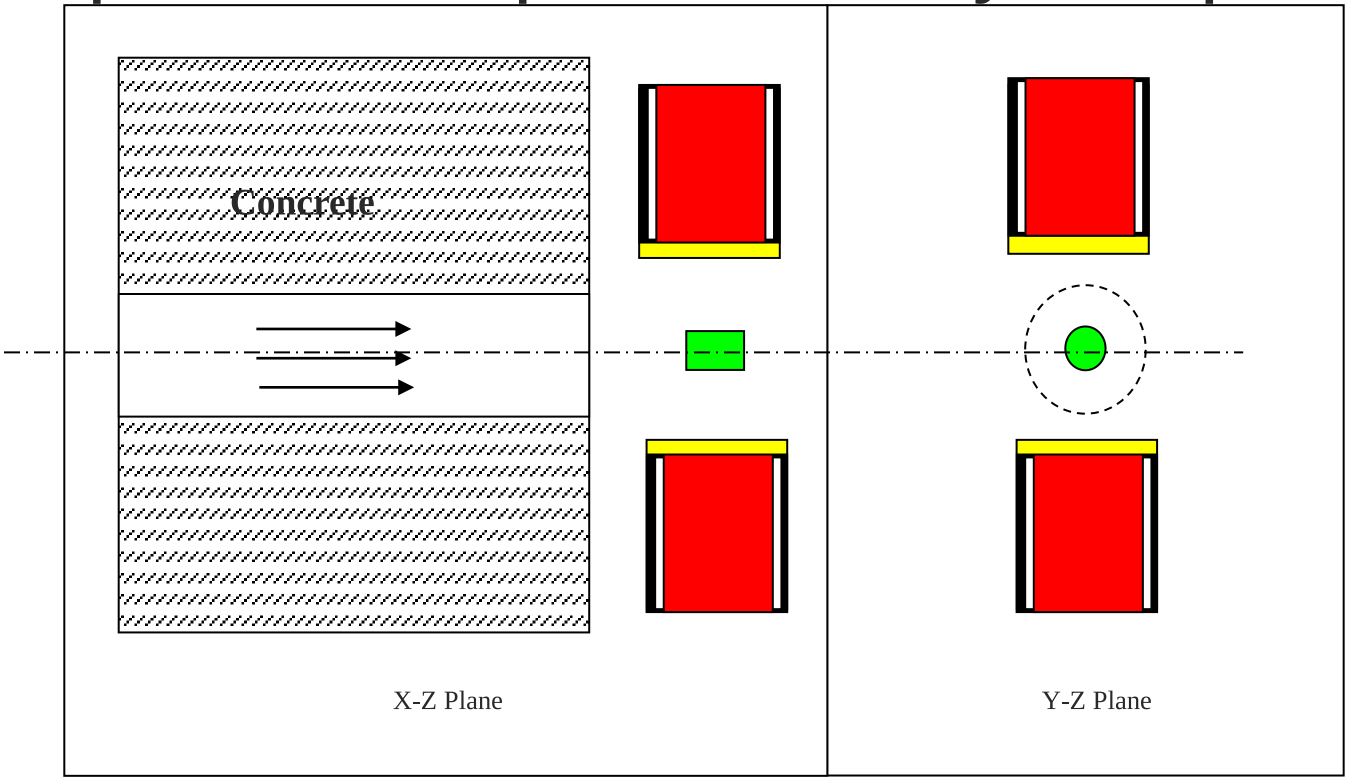
Benchmark Experiments

- Experiment 3 pure mercury sample



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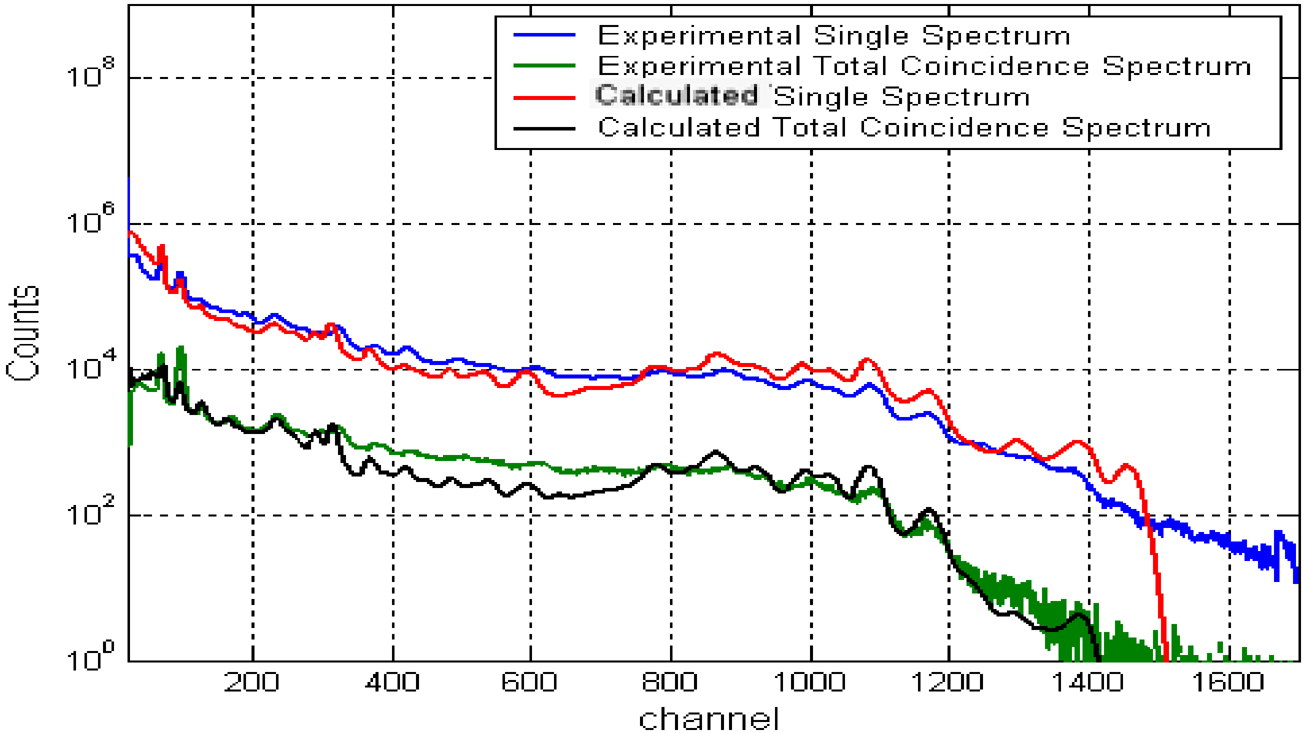
Benchmark Experiments



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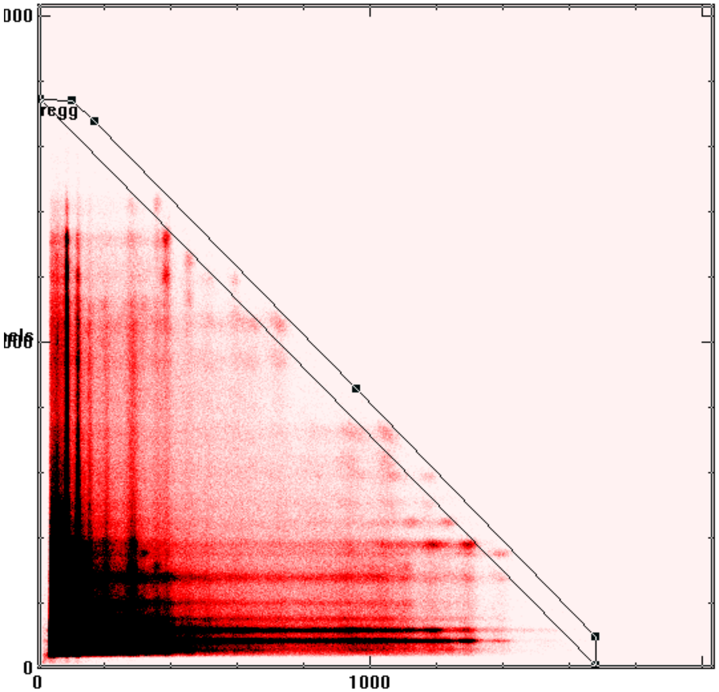
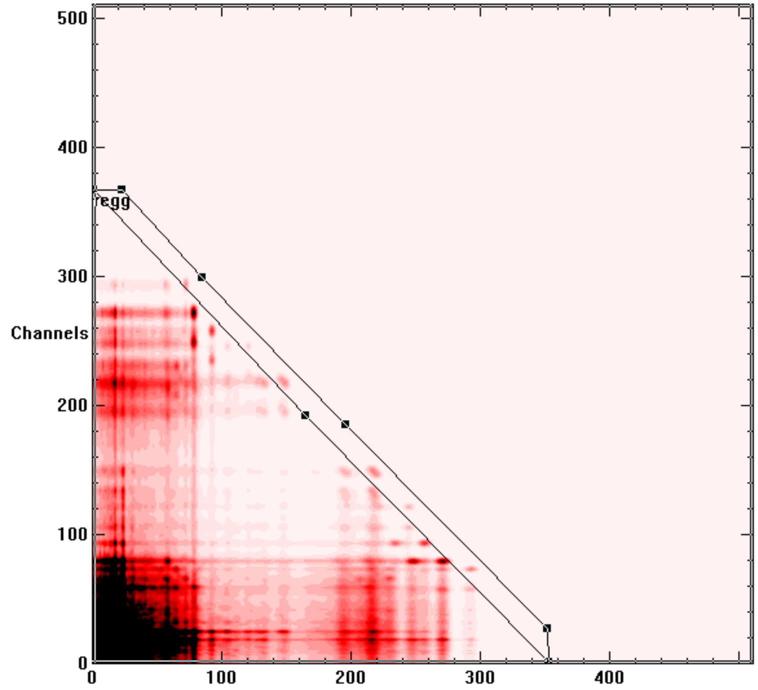
Benchmark Experiments





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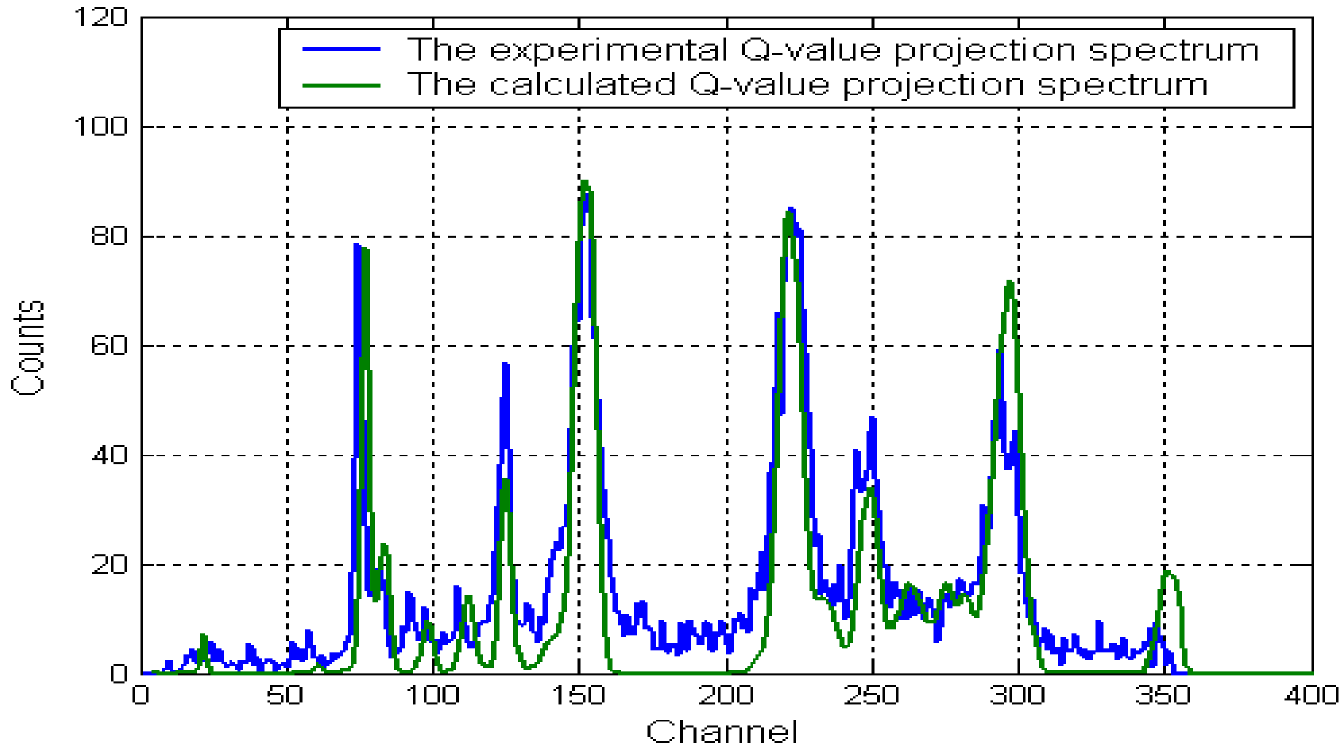
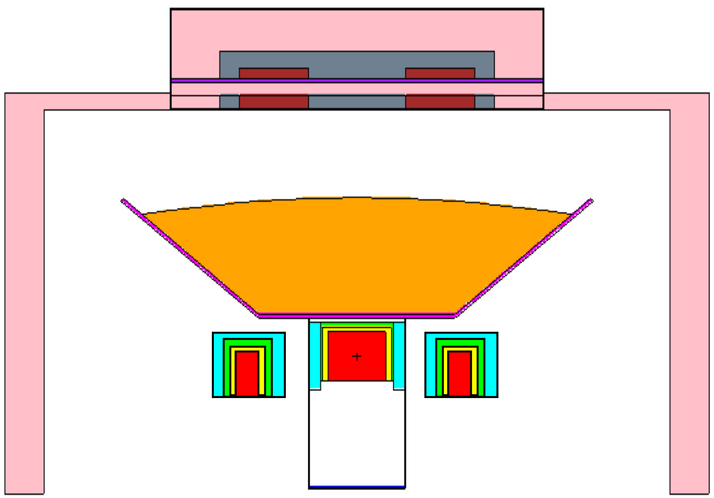
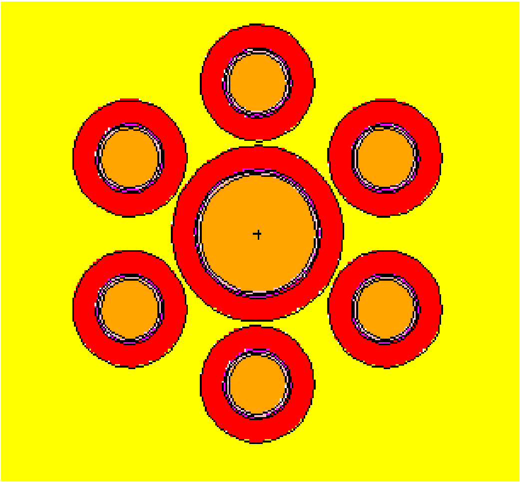
Benchmark Experiments



Optimization of CPGNAA application





Conclusion

- Coincidence PGNAA is a new developing technique and has already been approved that it can significantly reduce the interference and increase the accuracy of PGNAA analysis
- Code CEARCPG is the first specific MC code which can be used to simulate the coincidence spectra.
- Several benchmark experiments have been carried out to check the simulation results of CEARCPG. The results indicate that this code is accurate and very useful in the design for coincidence PGNAA device.

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