MCNP-CP, an Extended Version of a General Purpose Monte Carlo N-Particle Transport Code with Radionuclide Source and Coincidence / Anticoincidence Pulse Height Tally

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Outline

- Introduction
- MCNP-CP physics
- MCNP card extensions
- Applications
- Summary

Motivation

- Decay of radioactive nuclei and isomeric states usually represents a complex multi-stage atomic-nuclear process, which results in emission of **space and time correlated particles**: photons, β-particles, discrete energy electrons, and X-rays.

- Accurate prediction of a detection system response in measurements with such sources requires application of an **adequate source model**.

Restrictions of the standard MCNP

- Only one source particle per history is considered,
- Only source particles of particular type are considered within a calculation run, and
- There are no standard means for calculating pulse height distributions for the detection systems, which use coincidence / anticoincidence measurement techniques.

Background publications

- **A.N. Berlizov, V.V. Tryshyn** / ENSDF Based Radionuclide Source for MCNP // Proceedings of the International Conference on Supercomputing in Nuclear Applications, SNA'2003, 22-24 September 2003, Paris, France.
- **A.N. Berlizov** / An upgraded multidetector pulse height tally for MCNP // Proceedings of the Monte Carlo 2005 Topical Meeting, Chattanooga, USA, April 17-21, 2005, ISBN:0-89448-695-0, American Nuclear Society, Inc.
- **A.N. Berlizov** / MCNP-CP, a Correlated Particle Radiation Source Extension of a General Purpose Monte Carlo N-Particle Transport Code // Applied Modeling and Computations in Nuclear Science. T.M. Semkow, S. Pomme, and S.M. Jerome, Eds. ACS Symposium Series 945. American Chemical Society, Washington, DC, 2006, p.183-194.

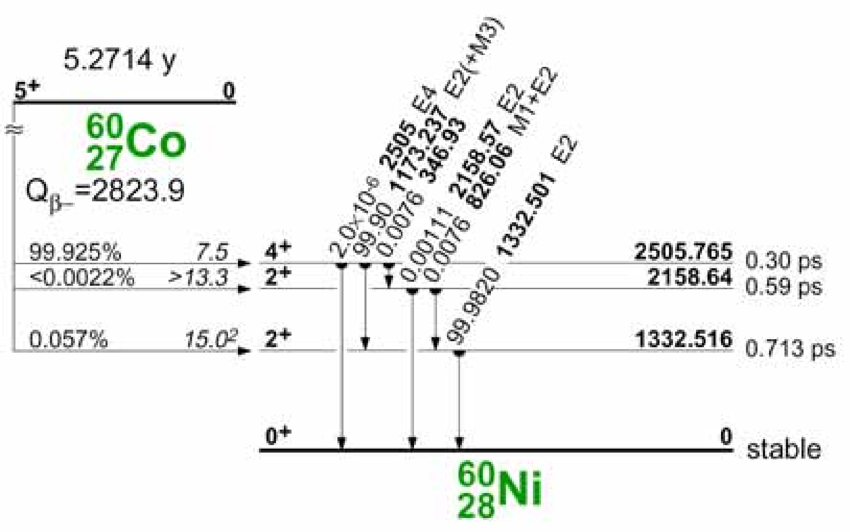
For modeling radionuclide source MCNP-CP uses:

- **Evaluated Nuclear Structure Data File ENSDF** as a basic source of information about decay properties of radionuclides.

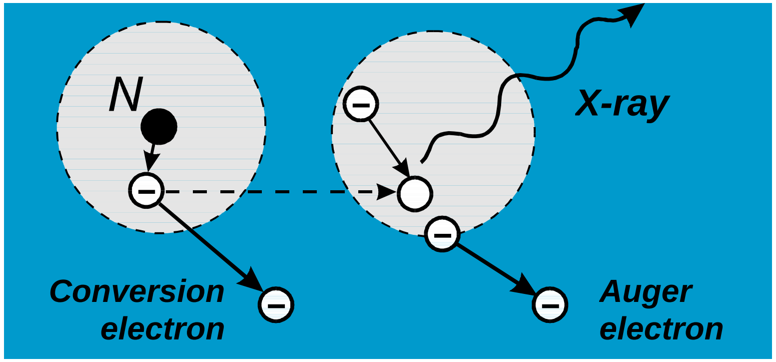
- **Known theoretical models and additional nuclear and atomic data** for simulating:
- spectral distributions of β-particles from β^--decay;
- vacancy creation on the atomic K-shell and $L_{1,2,3}$-subshells in the electron capture and internal conversion processes;
- emission of a pair of annihilation 511-keV photons in β^+-decay;
- Doppler shifting of annihilation photon energies and directions;
- intra-atomic transitions resulting in the emission of K- and LX-rays in single and double X-ray fluorescence, emission of K-LX and K-MX Auger-electrons;
- γ-γ angular correlations of cascade γ-rays.

Electromagnetic transitions

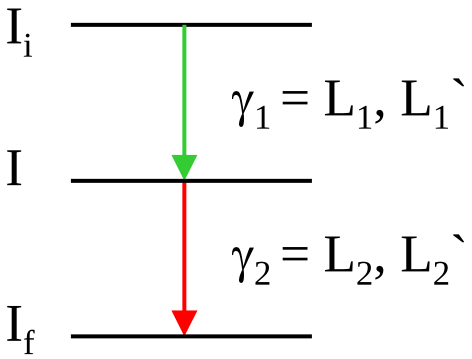
- Cascades of electromagnetic transitions are modeled based on the decay scheme information taken from the ENSDF data file.



- In each transition two competing decay modes are considered: the emission of a gamma-ray and the emission of a conversion electron from the atomic K-shells or $L_{1,2,3}$-subshells.



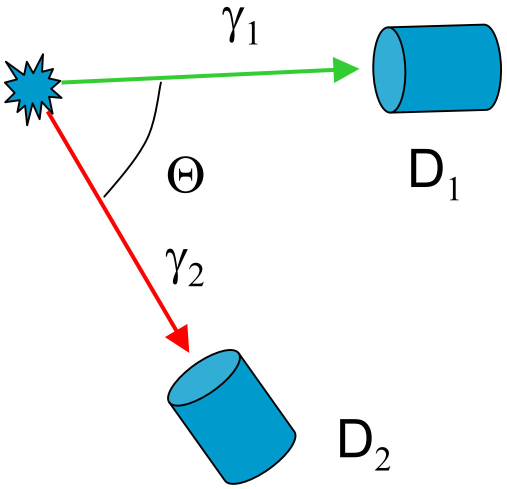
Angular correlations of cascade gamma-rays

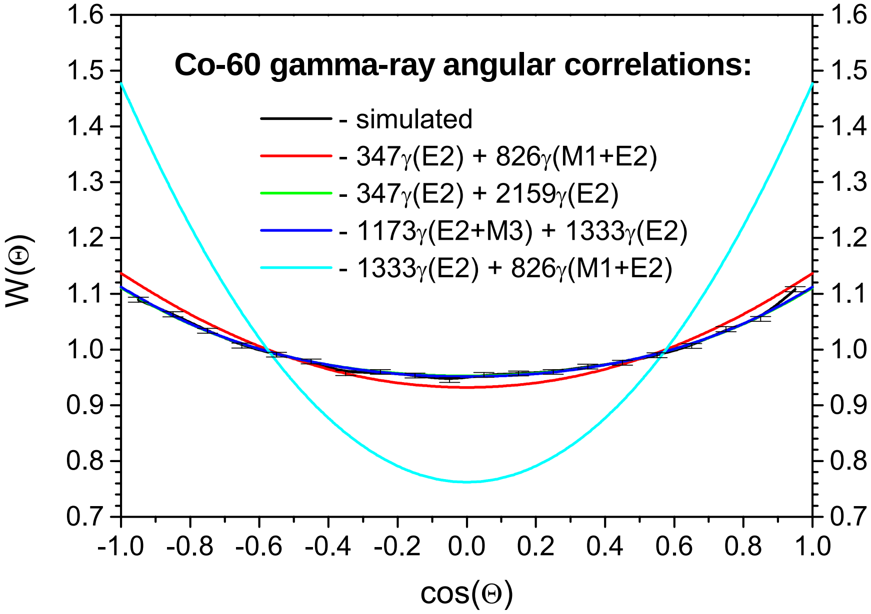


$$W(\Theta) = 1 + \sum_{k=2}^{k_{max}} A_{kk} P_k(\cos\Theta)$$

k – even integer number:

$$k_{max} = \min(L_1 + L_1', L_2 + L_2', 2I)$$





Modeling energy distributions of β⁻-particles

Beta spectrum:

$$dN_e(Q_\beta, T_e) \propto |M_{fi}|^2 \, (T_e(T_e + 2m_ec^2))^{1/2}(T_e + m_ec^2)(Q_\beta - T_e)^2 F(T_e, Z) \, dT_e$$

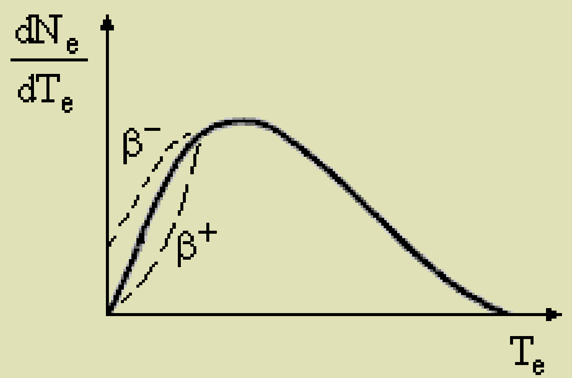
Nuclear matrix element:

$$M_{fi} = G\int \varphi_f^* \varphi_i \exp(-i(p+q)r/\hbar)dr$$

- non-unique transitions: $|M_{fi}|^2 \sim 1$

- unique transitions: $|M_{fi}|^2 \sim p^2+(Q_\beta-T_e)^2$

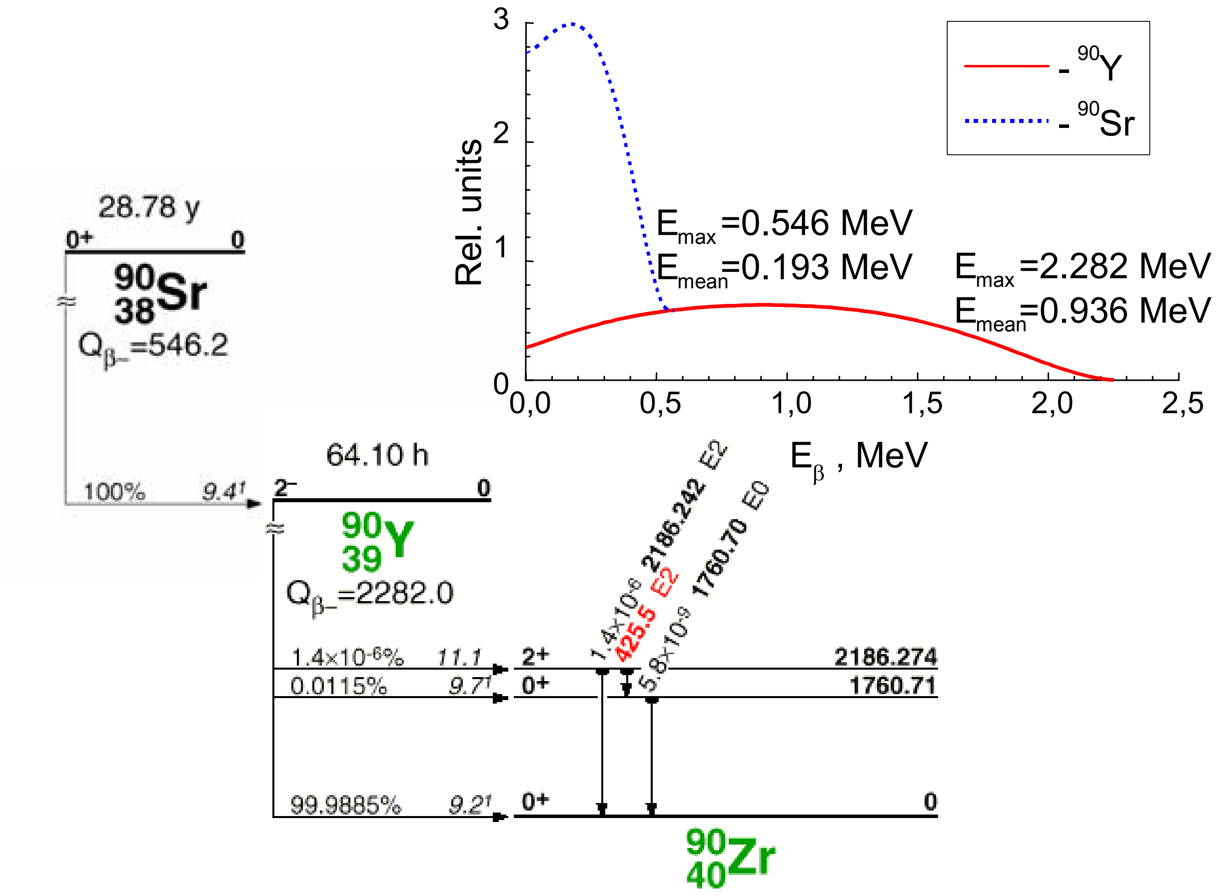
Coulomb interaction of a beta-particle with a nucleus:



Point nucleus approximation
(non-relativistic approach):

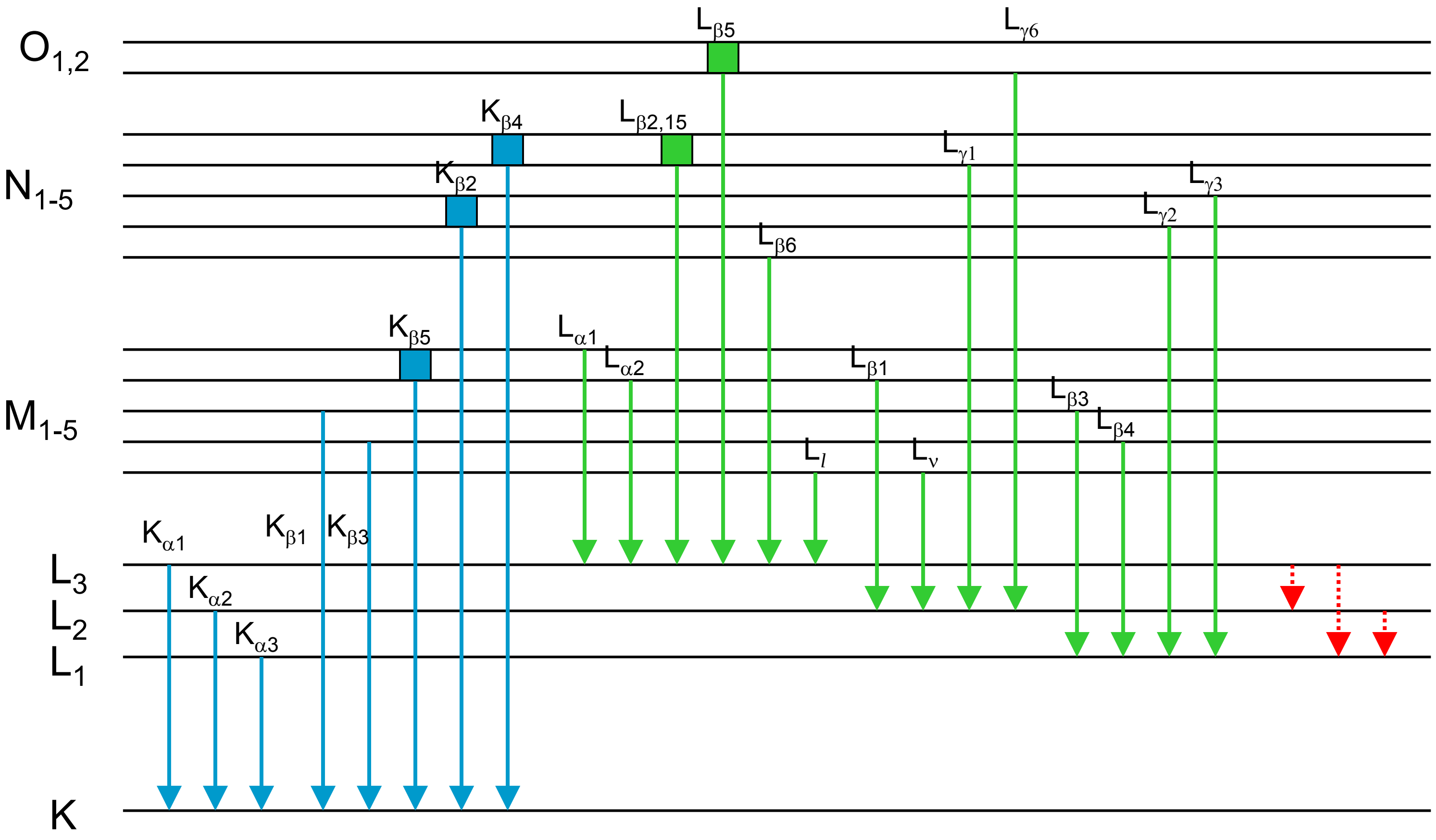
$$F(T_e, Z) = \frac{2\pi\eta}{1 - \exp(-2\pi\eta)} \qquad \eta = \pm\frac{\alpha Z(T_e + m_ec^2)}{pc}$$

β^--particle energy distributions: ^{90}Sr-^{90}Y source



Modeling of intra-atomic transitions

X-ray and Koster-Cronig transitions taken into consideration:



Emission of Auger electrons

Following 54 Auger transitions are taken into consideration:

K-L$_1$X: K-L$_1$L$_1$ K-L$_1$L$_2$ K-L$_1$M$_1$ K-L$_1$M$_2$ K-L$_1$M$_3$ K-L$_1$M$_4$ K-L$_1$M$_5$ K-L$_1$N$_1$ K-L$_1$N$_2$ K-L$_1$N$_3$ K-L$_1$O$_1$ K-L$_1$O$_2$ K-L$_1$O$_3$

K-L$_2$X: K-L$_2$L$_2$ K-L$_2$L$_3$ K-L$_2$M$_1$ K-L$_2$M$_2$ K-L$_2$M$_3$ K-L$_2$M$_4$ K-L$_2$M$_5$ K-L$_2$N$_1$ K-L$_2$N$_2$ K-L$_2$N$_3$ K-L$_2$O$_1$ K-L$_2$O$_3$

K-L$_3$X: K-L$_3$L$_3$ K-L$_3$M$_1$ K-L$_3$M$_2$ K-L$_3$M$_3$ K-L$_3$M$_4$ K-L$_3$M$_5$ K-L$_3$N$_1$ K-L$_3$N$_2$ K-L$_3$N$_3$ K-L$_3$N$_4$ K-L$_3$N$_5$ K-L$_3$O$_1$ K-L$_3$O$_2$ K-L$_3$O$_3$

K-M$_1$X: K-M$_1$M$_1$ K-M$_1$M$_2$ K-M$_1$M$_3$ K-M$_1$N$_1$ K-M$_1$N$_2$ K-M$_1$N$_3$

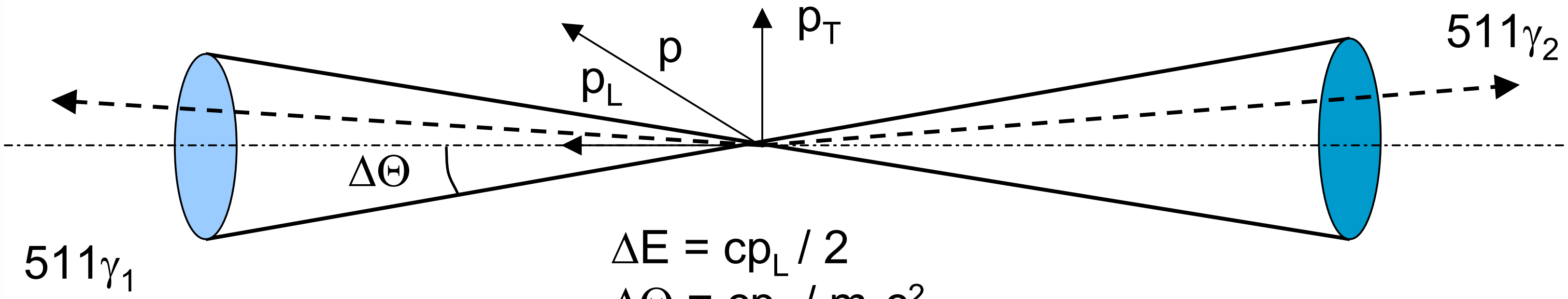
K-M$_2$X: K-M$_2$M$_3$ K-M$_2$N$_1$ K-M$_2$N$_3$

K-M$_3$X: K-M$_3$M$_3$ K-M$_3$M$_4$ K-M$_3$M$_5$ K-M$_3$N$_1$ K-M$_3$N$_2$ K-M$_3$N$_3$

Auger electron energies: $E(K\text{-}LX) = B_K - B_L - B_X$, $E(K\text{-}MX) = B_K - B_M - B_X$
Emission probabilities: *M.O. Krause* (*J. Phys. Chem. Ref. Data, 8 ,1979*)

Annihilation photon emission

- Probability of emission of a pair of annihilation 511-keV photons is evaluated assuming local deposition of kinetic energy of a positron and by neglecting the on-the-fly annihilation process.
- Energies and directions of the annihilation photons are subject to Doppler shifting in the course of simulation based on the evaluations of *Prochazka (Materials Structure, 8, No.2 (2001) 55)* :



$\Delta E = cp_L / 2$
$\Delta\Theta = cp_T / m_ec^2$

$E_{12} = 511 \pm \sigma_E$, $\sigma_E = 1$ keV
$\Theta = \pi \pm \sigma_\Theta$, $\sigma_\Theta = 2\,\Delta E / m_ec^2 = 0.0039$ radians (liquids and gases).

General source card extension

SDEF … ZAM=zzzaaam …

zzzaaam = zzz - atomic number (nucleus charge),
aaa - mass number, and
m - isomeric index of the radionuclide of interest.
… = standard SDEF card parameters specifying source location and geometry: CEL, SUR, X, Y, Z, POS, EXT, RAD, AXS, CCC.

Default: zzzaaam = 0000000, which results in standard SDEF card function.

Example: SDEF POS=0 0 0 ZAM=270600
^{60}Co point source (Z = 27, A = 60, M = ground state) located at the origin of a coordinate system

Source settings card

CPS RT IAS IGA IAN IKX ILX IBT ICE IAE IGG

RT = the correlated particle grouping time in shakes.
IAS = analog/semi-analog decay simulation flag.
IGA = decay gamma-ray emission flag.
IAN = annihilation photon emission flag.
IKX = KX-ray emission flag.
ILX = LX-ray emission flag.
IBT = beta-particles emission flag.
ICE = conversion electrons emission flag.
IAE = Auger electrons emission flag.
IGG = gamma-gamma angular correlation flag.

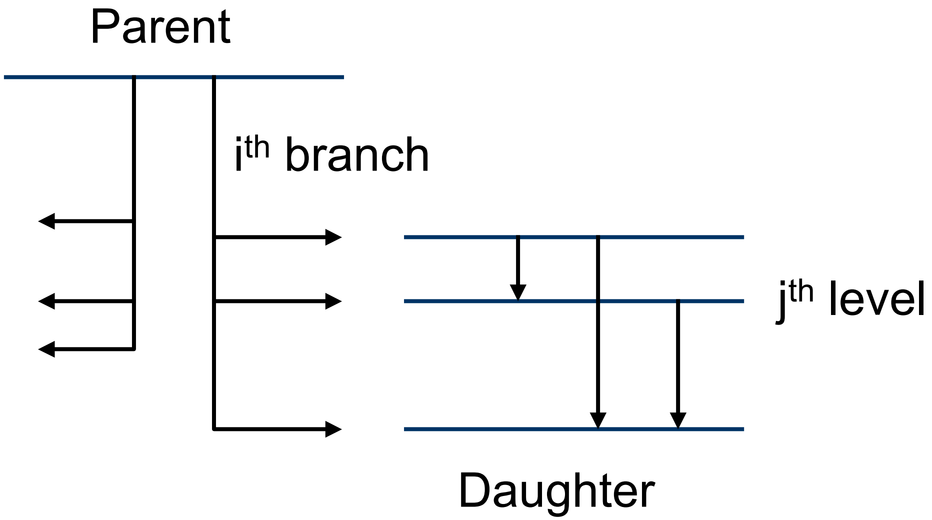
Default: RT=50 IAS=IGA=IAN=IKX=ILX=IBT=ICE=IAE=IGG=1.

Use: Use IGA through IAE entries to enable (0) or disable (1) emission of different types of particles. Zero value of IGG flag suppresses modeling of gamma-gamma angular correlations.

CPS card: Source simulation modes

- **RT > 0:** particles are grouped within the time intervals with length RT according to their emission times. Then each of the particle groups are tracked in different histories (one history per group), thus assuming no correlations between groups. This mode can be considered as a **realistic source mode**.
- **RT = 0:** all particles are considered within one group (and within one history) disregarding their emission times, the so called **forced correlation** case.
- **RT = -1:** particles are sampled in the same manner as it is done in two previous modes, but each particle is tracked in a separate history disregarding its emission time. This is so called **forced uncorrelated source mode**.
- **RT < 0 (RT ≠ -1):** all particles are sampled independently using per-decay probabilities. Tracking of particles is carried out in separate histories, one history per one particle. This is the case of **totally uncorrelated source**.

IAS flag: analog / semi-analog source simulation modes



Analog (IAS=1)
$P_{ij}=BR_i \cdot PP_j$
$wgt_{ij}=1$

Semi-analog (IAS=0)
$P_{ij}=1$
$wgt_{ij}=BR_i \cdot PP_j$

P_{ij} - probability of population of level “j” through decay branch “i”,
BR_i – branching ratio for decay branch “i”,
PP_j – population probability for level “j”,
wgt_{ij} - particle weights assigned when simulating the decay.

Extended pulse-height tally F8

Fn:p1 bin_1 bin_2 … bin_M

n = tally number (8, 18, 28 …).
p1 = P, E or P,E.
M = number of tally bins.
bin_i = *i*-th tally cell bin.

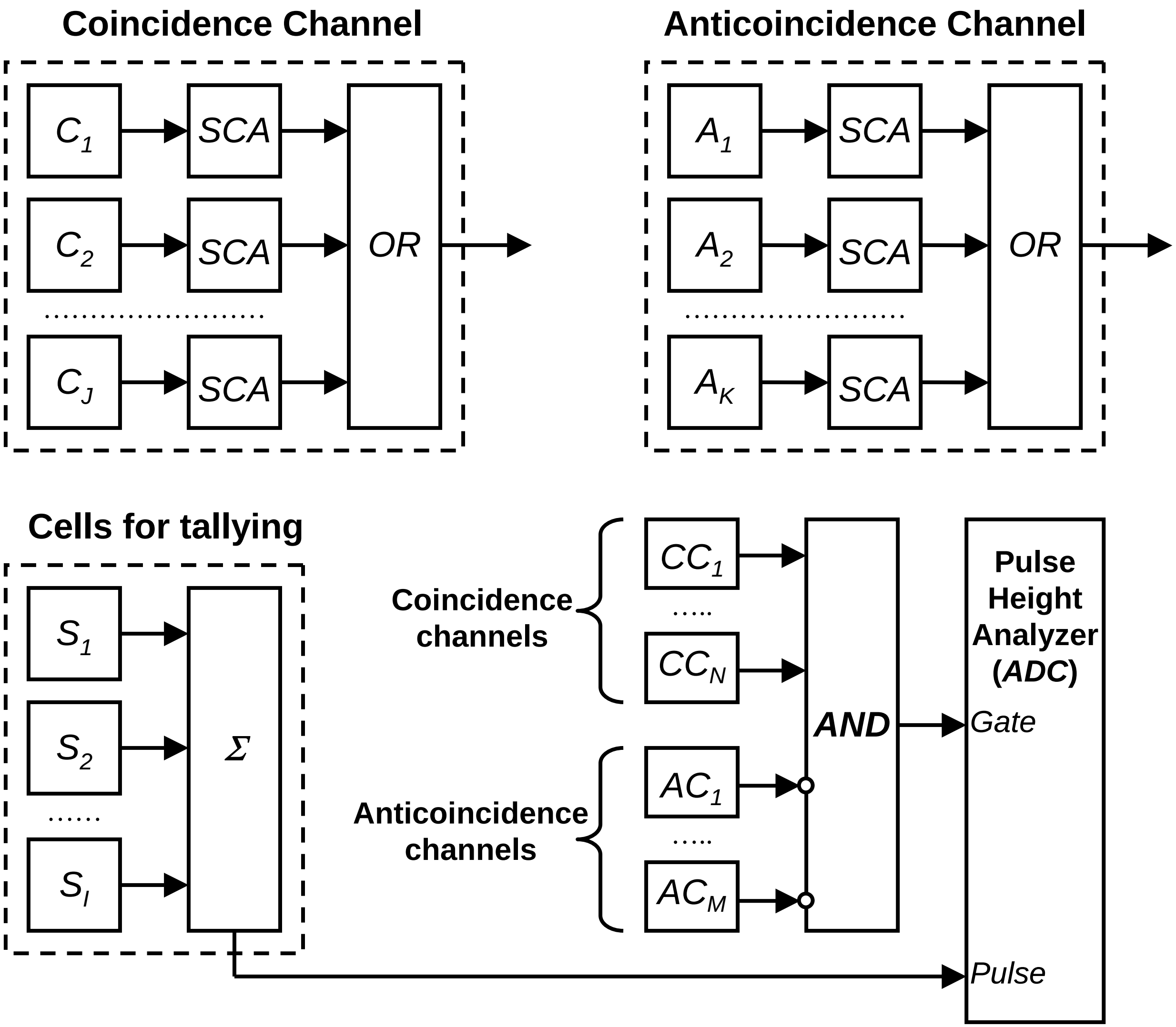
All standard formats of cell bins remained supported:

- single cell - bin = *S*, where S is problem number of cell for tallying;
- cell union - bin = $(S_1\ S_2\ \ldots\ S_N)$;
- rep. structure and lattice tally - bin = $((S_1\ S_2) < (C_1\ C_2[I_1\ \ldots\ I_2]) < (C_3\ C_4\ C_5))$.

New Coincidence / Anticoincidence tally bin format:

$$\mathbf{bin} = (\underbrace{(S_1 \ldots S_I)}_{\text{Cells for tallying}}\ \underbrace{+(C_{11} \ldots C_{1J1}) \ldots\ -(A_{11} \ldots A_{1K1}) \ldots}_{\text{Tallying condition}})$$

Logic of tallying of a coincidence / anticoincidence cell bin



MCNP-CP output

```
1decay branch: Eu-152  EC Sm-152 (13.54 y) -  72.08%      print table 210

Exited and ground level properties
--------------------------------------------------------------------------------------
   Level         Spin & Parity       Half          Transition intensities  *     Flag
 ##    E,keV   ENSDF2   Taken as     Life      Beta-    Beta+     EC      Alpha   **
--------------------------------------------------------------------------------------
  1     0.000      0+       0+      stable     0.0000   0.0000   0.0000   0.0000  A/NQ
  2   121.782      2+       2+     1.396 NS    0.0000   0.0110   0.7421   0.0000  A/NQ
  3   366.479      4+       4+       60 PS     0.0000   0.0028   0.9025   0.0000  A/NQ
  4   684.701      0+       0+                 0.0000   0.0000   0.0000   0.0000  A/NQ
  5   706.880      6+       6+                 0.0000   0.0000   0.0000   0.0000  A/NQ
  6   810.453      2+       2+        7 PS     0.0000   0.0000   1.3036   0.0000  A/NQ
  7   963.354      1-       1-                 0.0000   0.0000   0.0000   0.0000  A/NQ
  8  1022.966      4+       4+                 0.0000   0.0000   0.2377   0.0000  A/NQ
  9  1041.114      3-       3-        5 PS     0.0000   0.0000   0.0762   0.0000  A/NQ
 10  1085.883      2+       2+        4 PS     0.0000   0.0000  21.7903   0.0000  A/NQ
 11  1233.855      3+       3+        6 PS     0.0000   0.0000  17.4583   0.0000  A/NQ
 12  1292.757     (2+)      2+                 0.0000   0.0000   0.6598   0.0000  A/NQ
 13  1371.744      4+       4+                 0.0000   0.0000   0.8614   0.0000  A/NQ
 14  1529.794      2-       2-       27 FS     0.0000   0.0000  24.9892   0.0000  A/NQ
 15  1579.432      3-       3-                 0.0000   0.0000   2.0908   0.0000  A/NQ
 16  1612.780    4+,5-      4+                 0.0000   0.0000   0.0212   0.0000  A/Q
 17  1649.889      2-       2-                 0.0000   0.0000   0.9256   0.0000  A/NQ
 18  1730.240     (3-)      3-                 0.0000   0.0000   0.0424   0.0000  A/NQ
 19  1757.032    2+,3+      2+                 0.0000   0.0000   0.0471   0.0000  A/NQ
 20  1769.100      2+       2+                 0.0000   0.0000   0.0662   0.0000  A/NQ
--------------------------------------------------------------------------------------
* Intensities per 100 decays of a parent nucleus.
** Adopted, NonAdopted, Questionable or NonQuestionable level.
```

MCNP-CP output (cont'd)

```
Vacancies due to electron capture
--------------------------------------------------------------------------
  Level         Decay   Unique   Intensity of vacancies on atomic shells
 ##   E,keV    Q, keV    ness     K-shell   L1-shell   L2-shell   L3-shell
--------------------------------------------------------------------------
 1     0.000  1874.300          0.00e+000  0.00e+000  0.00e+000  0.00e+000
 2   121.782  1752.518          6.25e-001  8.78e-002  3.40e-003  5.42e-005
 3   366.479  1507.821          7.59e-001  1.07e-001  4.15e-003  8.33e-005
 4   684.701  1189.599          0.00e+000  0.00e+000  0.00e+000  0.00e+000
 5   706.880  1167.420          0.00e+000  0.00e+000  0.00e+000  0.00e+000
 6   810.453  1063.847          1.09e+000  1.56e-001  6.05e-003  2.00e-004
 7   963.354   910.946          0.00e+000  0.00e+000  0.00e+000  0.00e+000
 8  1022.966   851.334          1.99e-001  2.87e-002  1.11e-003  4.93e-005
 9  1041.114   833.186          6.39e-002  9.20e-003  3.57e-004  1.63e-005
10  1085.883   788.417          1.83e+001  2.64e+000  1.02e-001  4.99e-003
11  1233.855   640.445          1.46e+001  2.13e+000  8.24e-002  5.14e-003
12  1292.757   581.543          5.52e-001  8.06e-002  3.12e-003  2.17e-004
13  1371.744   502.556          7.20e-001  1.06e-001  4.10e-003  3.31e-004
14  1529.794   344.506          2.08e+001  3.11e+000  1.20e-001  1.37e-002
15  1579.432   294.868          1.74e+000  2.61e-001  1.01e-002  1.30e-003
16  1612.780   261.520          1.76e-002  2.65e-003  1.03e-004  1.44e-005
17  1649.889   224.411          7.69e-001  1.17e-001  4.52e-003  7.01e-004
18  1730.240   144.060          3.51e-002  5.40e-003  2.10e-004  4.12e-005
19  1757.032   117.268          3.90e-002  6.03e-003  2.34e-004  5.01e-005
20  1769.100   105.200          5.47e-002  8.49e-003  3.29e-004  7.33e-005
--------------------------------------------------------------------------
 T O T A L :                    6.04e+001  8.84e+000  3.43e-001  2.70e-002
--------------------------------------------------------------------------
* Intensities per 100 decays of a parent nucleus.
```

MCNP-CP output (cont’d)

```
Properties of electromagnetic transitions
 --------------------------------------------------------------------------
 Transition     Level indexes     Multipolarity        Mixing       Gammas
  ##   E,keV    init  ->  fin   ENSDF2   Taken as      ratio          *
 --------------------------------------------------------------------------
   1   121.782    2       1        E2        E2       0.00000      28.65984
   2   244.697    3       2        E2        E2       0.00000       7.60451
   3   562.930    4       2        E2        E2       0.00000       0.00268
   4   340.400    5       3        E2        E2       0.00000       0.03651
   5   125.690    6       4       [E2]       E2       0.00000       0.01611
   6   443.965    6       3       (E2)       E2       0.00000       0.32748
   7   688.670    6       2     E2+M1+E0     M1       0.00000       0.85896
   8   810.451    6       1       (E2)       E2       0.00000       0.32050
   9   841.570    7       2        E1        E1       0.00000       0.16642
  10   963.390    7       1        E1        E1       0.00000       0.13529
  11   212.568    8       6        E2        E2       0.00000       0.01989
  12   316.200    8       5       (E2)       E2       0.00000       0.00215
  13   656.487    8       3    E2+M1+E0      M1       0.00000       0.14522
  14   901.181    8       2        E2        E2       0.00000       0.08616
  15   674.675    9       3        E1        E1       0.00000       0.17287
  16   919.330    9       2        E1        E1       0.00000       0.42787
  17   275.449   10       6       (M1)       M1       0.00000       0.03355
  18   719.349   10       3       (E2)       E2       0.00000       0.27916
  19   964.079   10       2   E2+M1(+E0)   M1+E2     -9.30000      14.64532
  20  1085.869   10       1        E2        E2       0.00000      10.23508
  21   148.010   11      10     [M1+E2]      M1       0.00000       0.03731
 ...  ........  ...     ...      ......    ......     .......      ........
---------------------------------------------------------------------------
 * Intensities per 100 decays of a parent nucleus.
```

MCNP-CP output (cont'd)

```
Internal conversion coefficients
-----------------------------------------------------------------------------------------------
Transition       Total         K-shell            L-shell         Calculated ICC for subshells*
 ##   E,keV     ENSDF2     ENSDF2   calc.*    ENSDF2    calc.*      L1        L2        L3
-----------------------------------------------------------------------------------------------
  1   121.782 1.17e+000 6.85e-001 6.85e-001 3.74e-001 3.74e-001 6.39e-002 1.55e-001 1.54e-001
  2   244.697 1.08e-001 8.13e-002 8.13e-002 2.08e-002 2.08e-002 8.76e-003 6.79e-003 5.29e-003
  3   562.930 9.50e-003 7.80e-003 7.80e-003 1.28e-003 1.28e-003 9.33e-004 2.21e-004 1.27e-004
  4   340.400 3.84e-002 3.04e-002 3.04e-002 6.26e-003 6.26e-003 3.44e-003 1.67e-003 1.14e-003
  5   125.690 1.04e+000 6.24e-001 6.24e-001 3.25e-001 3.25e-001 5.86e-002 1.34e-001 1.32e-001
  6   443.965 1.78e-002 1.44e-002 1.44e-002 2.60e-003 2.60e-003 1.69e-003 5.62e-004 3.49e-004
  7   688.670 4.34e-002 3.59e-002 8.42e-003 4.97e-003 1.13e-003 1.07e-003 5.58e-005 1.08e-005
  8   810.451 3.96e-003 3.32e-003 3.32e-003 4.90e-004 4.87e-004 4.01e-004 5.66e-005 2.98e-005
  9   841.570 1.44e-003 1.23e-003 1.23e-003 1.59e-004 1.59e-004 1.46e-004 6.11e-006 6.96e-006
 10   963.390 1.11e-003 9.50e-004 9.50e-004 1.22e-004 1.22e-004 1.13e-004 4.24e-006 4.90e-006
 11   212.568 1.71e-001 1.25e-001 1.25e-001 3.60e-002 3.60e-002 1.31e-002 1.26e-002 1.03e-002
 12   316.200 4.80e-002 3.76e-002 3.77e-002 8.11e-003 8.11e-003 4.23e-003 2.28e-003 1.60e-003
 13   656.487 5.68e-002 4.97e-002 9.47e-003 6.80e-003 1.28e-003 1.20e-003 6.39e-005 1.22e-005
 14   901.181 3.14e-003 2.63e-003 2.63e-003 3.80e-004 3.77e-004 3.19e-004 3.88e-005 2.01e-005
 15   674.675 2.26e-003 1.92e-003 1.93e-003 2.52e-004 2.52e-004 2.28e-004 1.13e-005 1.27e-005
 16   919.330 1.22e-003 1.04e-003 1.04e-003 1.34e-004 1.34e-004 1.23e-004 4.81e-006 5.53e-006
 17   275.449 1.03e-001 8.75e-002 8.75e-002 1.22e-002 1.22e-002 1.13e-002 7.73e-004 1.37e-004
 18   719.349 5.21e-003 4.34e-003 4.34e-003 6.60e-004 6.58e-004 5.24e-004 8.74e-005 4.71e-005
 19   964.079 2.73e-003 2.30e-003 2.30e-003 3.20e-004 3.25e-004 2.79e-004 3.05e-005 1.56e-005
 20  1085.869 2.11e-003 1.78e-003 1.78e-003 2.50e-004 2.47e-004 2.16e-004 2.04e-005 1.04e-005
 21   148.010 5.77e-001 4.30e-001 4.80e-001 1.10e-001 6.75e-002 6.19e-002 4.77e-003 8.56e-004
 22   423.450 2.70e-002 2.20e-002 2.85e-002 3.50e-003 3.90e-003 3.63e-003 2.23e-004 4.03e-005
 23   867.373 3.46e-003 2.90e-003 2.90e-003 4.20e-004 4.19e-004 3.52e-004 4.41e-005 2.27e-005
 24  1112.069 2.02e-003 1.71e-003 1.71e-003 2.40e-004 2.36e-004 2.08e-004 1.87e-005 9.46e-006
 ... ........ ......... ......... ......... ......... ......... ......... ......... .........
-----------------------------------------------------------------------------------------------
* Calculated are from Band et al for Z=3,6,14-29 and Hager-Seltzer for Z > 29.
x denotes measured ENSDF2 values.
```

MCNP-CP output (cont'd)

KX-ray and associated Auger transition intensities

```
-------------------------------------------------------------------------------------
            K-shell X-rays                             Auger electrons
Notation  E, keV  Intensity*  Intensity**  Notation   E, keV  Intensity*  Intensity**
-------------------------------------------------------------------------------------
 Ka1     40.1180  4.820e+001  3.894e+001    K-L3L3   33.4018  7.720e-001  6.237e-001
 Ka2     39.5224  2.660e+001  2.149e+001    K-L2L2   32.2106  7.980e-002  6.447e-002
 Ka3     39.0974  6.750e-003  5.453e-003    K-L2L3   32.8062  1.590e+000  1.285e+000
 Kb1     45.4144  9.120e+000  7.368e+000    K-L1L1   31.3606  6.140e-001  4.961e-001
 Kb2     46.5777  3.010e+000  2.432e+000    K-L1L2   31.7856  7.940e-001  6.415e-001
 Kb3     45.2935  4.710e+000  3.805e+000    K-L1L3   32.3812  7.750e-001  6.261e-001
 Kb4     46.7052  1.140e+000  9.210e-001
 Kb5     45.7411  1.350e-001  1.091e-001
-------------------------------------------------------------------------------------
* Intensities are per 100 K-shell vacancies.
** Intensities per 100 decays of a parent nucleus.
```

LX-ray energies and intensities

```
--------------------------------------------------------------------
 L-shell X-rays       Intensity per 100 vacancies on      Intensity
Notation  E, keV   L1-subshell  L2-subshell  L3-subshell      *
--------------------------------------------------------------------
 La1     5.6360   3.330e+000   1.520e+000   1.010e+001   5.499e+000
 Lb2     6.5872   7.030e-001   3.200e-001   2.140e+000   1.165e+000
 La2     5.6102   3.700e-001   1.690e-001   1.120e+000   6.105e-001
 Lb5     0.0000   0.000e+000   0.000e+000   0.000e+000   0.000e+000
 Lb6     6.3705   3.100e-002   1.410e-002   9.420e-002   5.115e-002
 Ll      4.9934   1.390e-001   6.310e-002   4.210e-001   2.284e-001
 Lb1     6.2058   2.240e+000   1.180e+001   0.000e+000   3.641e+000
 Ln      5.5890   5.480e-002   2.880e-001   0.000e+000   8.919e-002
 Lg1     7.1828   3.690e-001   1.940e+000   0.000e+000   6.008e-001
 Lg6     0.0000   0.000e+000   0.000e+000   0.000e+000   0.000e+000
 Lb3     6.3170   3.470e+000   0.000e+000   0.000e+000   4.720e-001
 Lb4     6.1961   2.080e+000   0.000e+000   0.000e+000   2.831e-001
 Lg2     7.4712   6.410e-001   0.000e+000   0.000e+000   8.724e-002
 Lg3     7.4894   9.120e-001   0.000e+000   0.000e+000   1.242e-001
--------------------------------------------------------------------
* Intensities per 100 decays of a parent nucleus.
```

MCNP-CP output (cont'd)

```
Gamma-gamma true coincidence table*.
 -------------------------------------------------------------------------------------------
 ##   E, keV  Ten the most intense coinciding gamma-rays, keV
 -------------------------------------------------------------------------------------------
 1    121.78 1408.01  964.10 1112.07  244.70  867.38  443.91 1212.95  688.67 1005.26 1457.65
 2    125.75  121.78  443.91  564.01  295.94  416.03  768.98  719.34  147.97  275.43  493.55
 3    147.97  121.78  964.10 1085.88  244.70  688.67  295.94  443.97  810.45  719.40  416.03
 4    207.69  121.78  964.10 1085.88  244.70  688.67 1005.26  919.33  443.97  810.45  719.40
 5    212.51  121.78  244.70  688.67  443.97  810.45  556.47  125.75  269.79  357.13  562.92
 6    239.31  121.78 1408.01  964.10 1112.07 1085.88  244.70  867.38  443.91  688.67  295.94
 7    244.70  121.78  867.38  443.91 1212.95 1005.26  564.01  295.94  488.68  443.97  719.40
 8    251.64  121.78  244.70  919.33  674.63  357.13
 9    269.79  121.78  244.70  688.67  443.97  810.45  656.49  901.18  340.40  212.51  125.75
 10   275.43  121.78  244.70  443.91  688.67  564.01  295.94  443.97  810.45  416.03  147.97
 11   285.86  121.78  964.10 1085.88  244.70  688.67  443.97  810.45  719.40  275.43  125.75
 12   295.94  121.78  964.10 1112.07 1085.88  244.70  867.38  688.67  443.97  810.45  719.40
 13   316.09  121.78  244.70  340.40  556.47  269.79  357.13
 14   329.40  121.78  841.57  963.35  357.13
 15   330.63  121.78  244.70  919.33  674.63  207.69  385.29
 16   340.40  121.78  244.70  556.47  664.86  905.90  269.79  207.69  385.29  357.13  316.09
 17   357.13  121.78  244.70  688.67  919.33  443.97  810.45  926.28  674.63  841.57  656.49
 18   385.29  121.78  964.10 1085.88  244.70  688.67 1005.26  919.33  443.97  810.45  719.40
 19   416.03  121.78  964.10 1112.07 1085.88  244.70  867.38  688.67  443.97  810.45  719.40
 20   423.40  121.78  244.70  688.67  295.94  443.97  810.45  416.03  125.75  523.18  496.39
 21   443.97  121.78  244.70  443.91  564.01  295.94  416.03  768.98  719.34  147.97  275.43
 22   443.91  121.78  964.10 1085.88  244.70  688.67  443.97  810.45  719.40  275.43  125.75
 23   482.30  121.78  244.70  688.67  443.97  810.45  125.75  357.13  562.92
 24   488.68  121.78  244.70  919.33  674.63  239.31
 25   493.55  121.78  964.10 1085.88  244.70  688.67  443.97  810.45  719.40  275.43  125.75
 ... ........ ......... ......... ......... ......... ......... ......... ......... .........
-------------------------------------------------------------------------------------------
 *    500.000 ns resolution time was assumed.
```

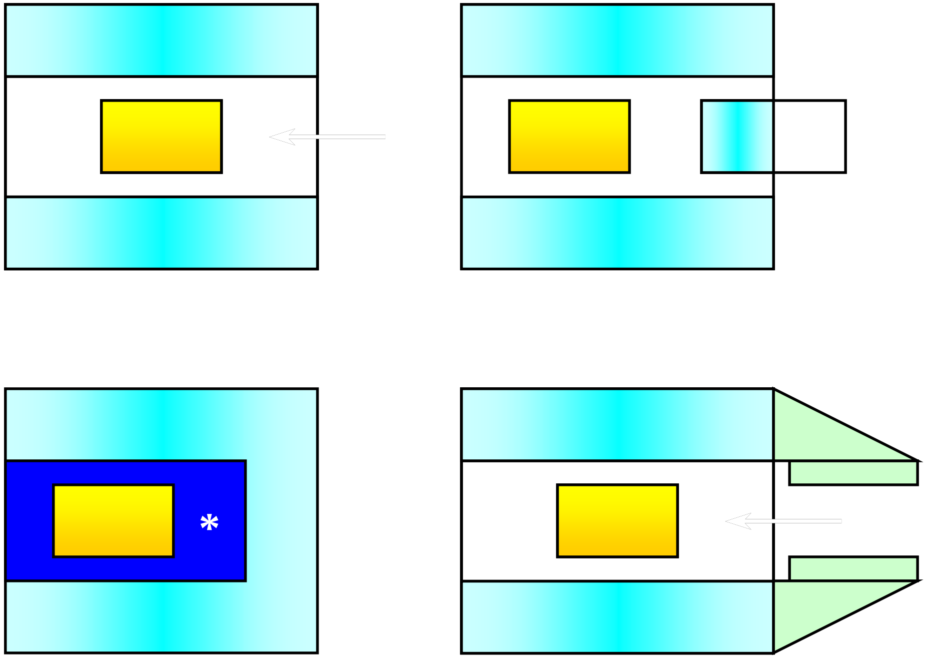
MCNP-CP output (cont’d)

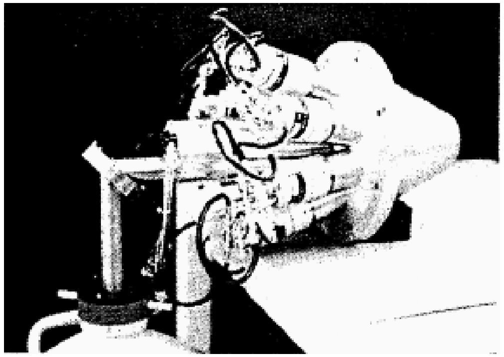
```
Sum peaks predictions (arranged by intensity).
------------------------------------------------------------------
##  Sum-Peak, keV  Pair of gamma-rays  Intensity product  Single
------------------------------------------------------------------
1     1529.79       121.78 + 1408.01       6.04e-002        No*
2     1233.86       121.78 + 1112.07       3.92e-002        No*
3      366.48       121.78 +  244.70       2.18e-002        Yes
4      989.16       121.78 +  867.38       1.22e-002        Yes
5      565.69       121.78 +  443.91       8.11e-003        Yes
6     1334.73       121.78 + 1212.95       4.09e-003        Yes
7     1529.79       443.91 + 1085.88       2.90e-003        No*
8      688.61       244.70 +  443.91       2.15e-003        Yes
9     1127.05       121.78 + 1005.26       1.86e-003        Yes
10    1579.43       121.78 + 1457.65       1.44e-003        No*
11     685.79       121.78 +  564.01       1.41e-003        Yes
12     417.72       121.78 +  295.94       1.28e-003        Yes
13    1041.11       121.78 +  919.33       1.23e-003        Yes
14     610.46       121.78 +  488.68       1.20e-003        Yes
15     565.76       121.78 +  443.97       9.39e-004        Yes
16    1649.89       121.78 + 1528.11       8.09e-004        No*
17     841.19       121.78 +  719.40       8.00e-004        Yes
18    1048.06       121.78 +  926.28       7.98e-004        Yes
19    1260.04       295.94 +  964.10       6.56e-004        Yes
....................................................        **
------------------------------------------------------------------
* Pair with the largest intensity product indicated.
**No pairs differing by > 100 times in intensity product included.
```

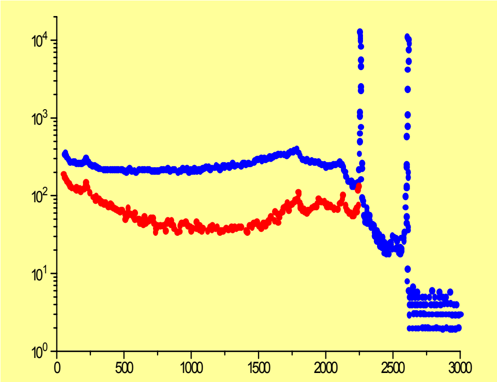
Possible applications

Calculation of characteristics and optimization of construction of detectors and detector systems:

- Single crystal spectrometers
- Pair Gamma-Spectrometers
- Phoswich detectors
- Compton/Escape Suppression Spectrometers



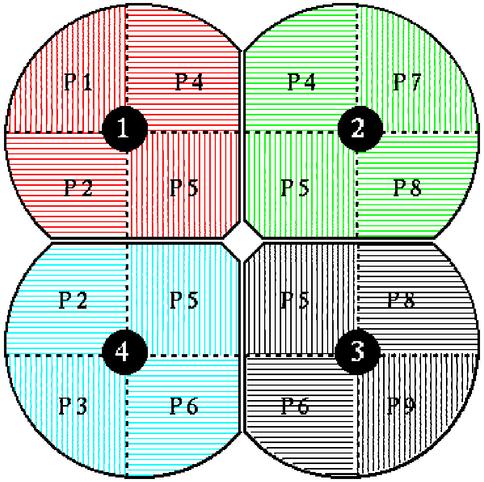




Possible applications (cont'd)

CLOVER segmented detector

NPRG at Liverpool, UK

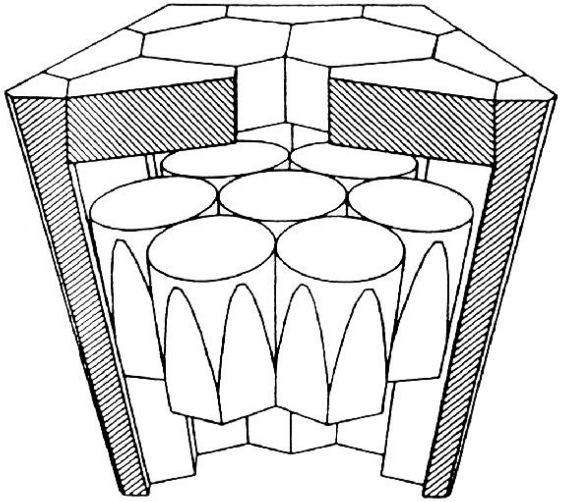


4 coaxial n-type Germanium crystals arranged like a four leaf clover. Outer p-type contact of each crystal segmented longitudinally, splitting each crystal into four quadrants.

http://ns.ph.liv.ac.uk/

CLUSTER detector

FZ Rossendorf, Germany



The detector comprises seven individually encapsulated HPGe crystals of about 60 % efficiency in a common cryostat surrounded by an escape-suppression shield consisting of 18 optically isolated BGO scintillator crystals.

http://www.fz-rossendorf.de/

Possible applications (cont'd)

GAMMASPHERE

Argonne National Laboratory, USA

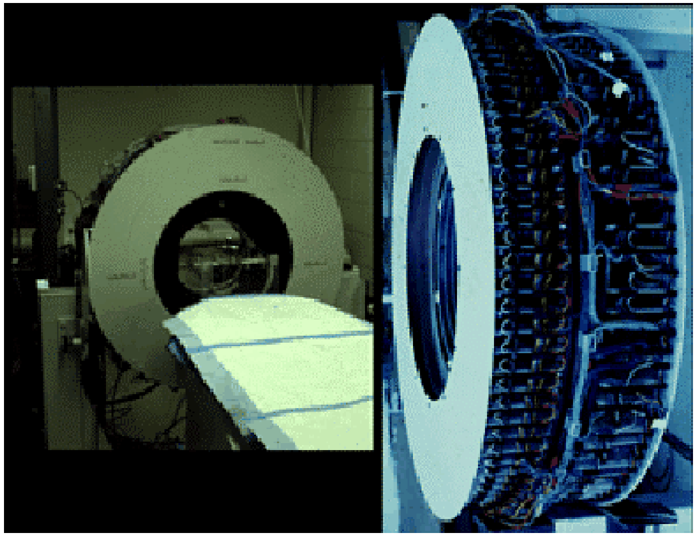
The array consists of 110 large volume, high purity germanium detectors, each in a BGO (Bismuth Germanate) compton suppression shield.

http://www-gam.lbl.gov/
http://www.phy.anl.gov/gammasphere/

ANL Physics Division

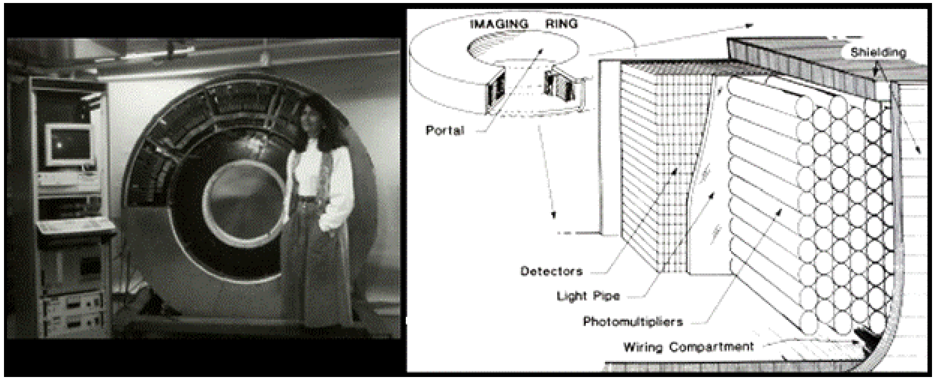
Possible applications (cont'd)

Nuclear Medical Imaging with Positron emission tomography (PET)



PCR-I, a single ring positron emission tomograph.

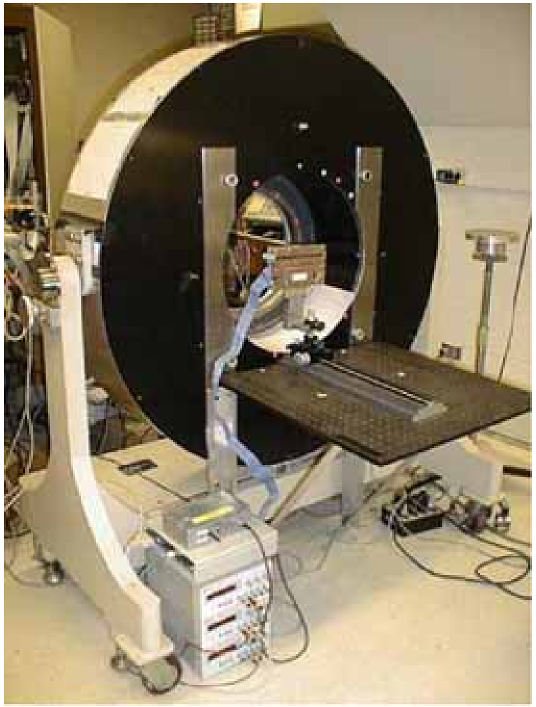
Source: A HISTORY OF POSITRON IMAGING
by Gordon L. Brownell,
Massachusetts Institute of Technology



PCR-II, a cylindrical positron emission tomograph.

Possible applications (cont'd)

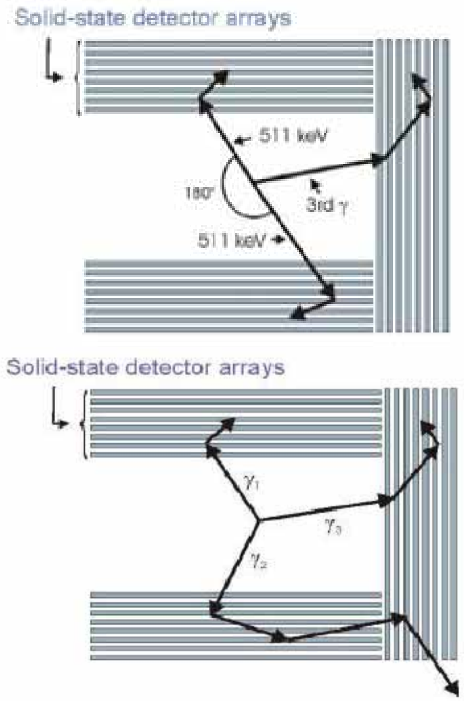
Compton Imaging System



Ring Compton camera. Scatter detector: 3×3 cm^2 silicon pad detectors. Absorption detector: Each of eleven detector modules is nominally composed of 44 NaI(Tl) bars.

Source: Compton Imaging System Development and Performance Assessment by Chia-ho Hua, University of Michigan, Ph.D. dissertation, 2000

Coincident Compton Imaging



Coincident Compton imager uses a positron emitting radionuclide accompanied by an additional γ-ray (top) or 3-gamma cascade (bottom)

Source: Coincident Compton Nuclear Medical Imager by James D. Kurfess and Bernard F. Phlips Naval Research Laboratory, Washington, DC USA

Possible applications (cont'd)

NDA techniques: Multi-Detector Analysis System for Spent Nuclear Fuel

Prototype MDAS has 68 detectors; 20 HPGe for gamma-ray detection and 48 liquid scintillator detectors for neutron detection.

Advantages: fast coincidence methods, list-mode data, gamma-ray coincidence, neutron coincidence, pulse-shape discrimination, detector arrays, and data acquisition and analysis.

Source: Using New Fission Data with the Multi-Detector Analysis System for Spent Nuclear Fuel by J.D. Cole et al., INEEL, USA

INEEL
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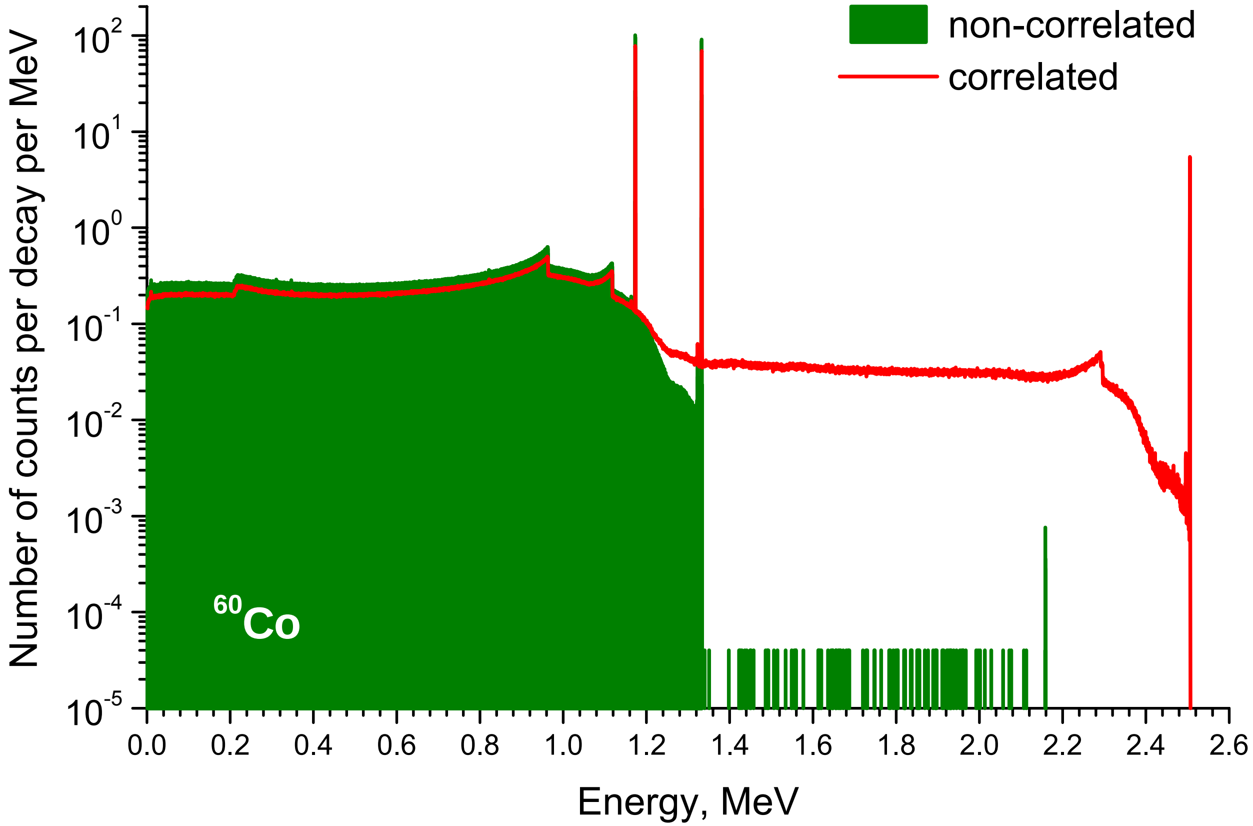
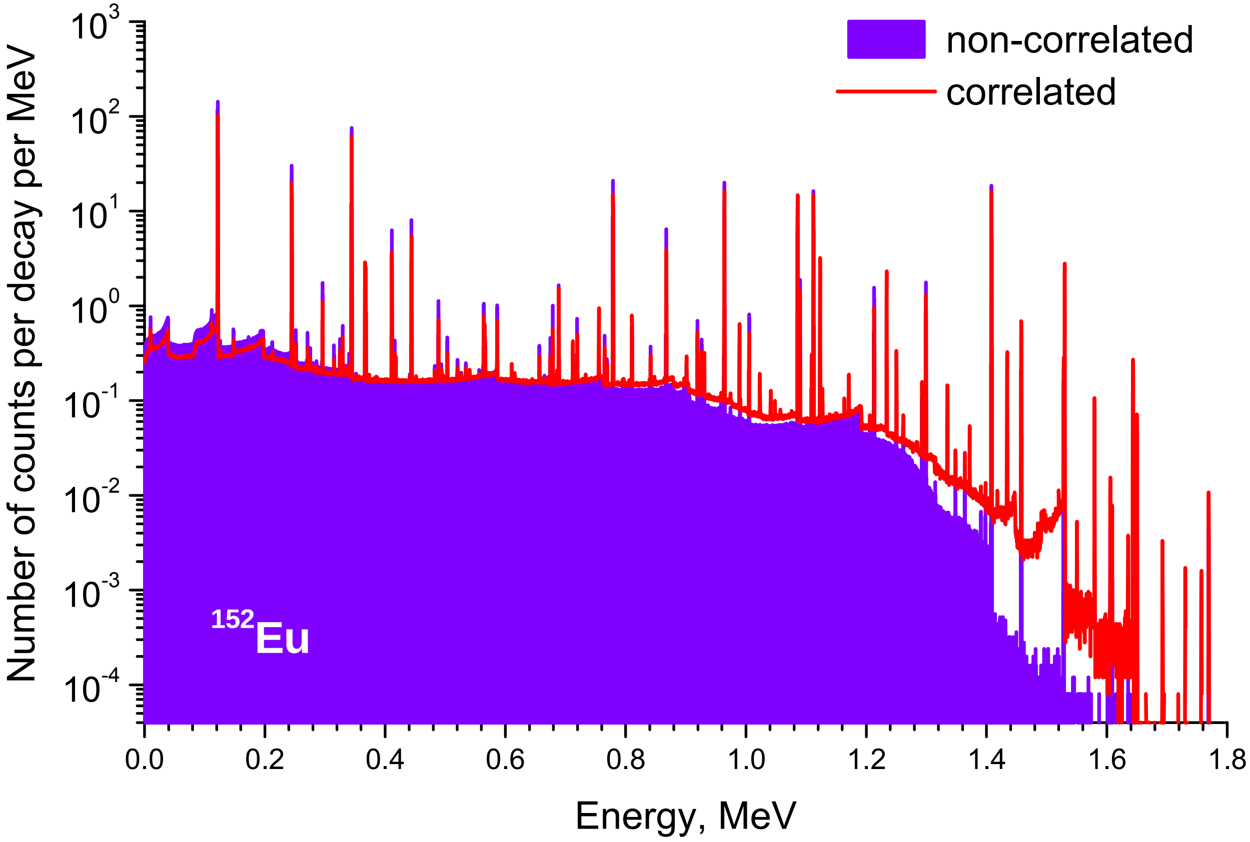
and Engineering Solutions

Coaxial 60% HPGe with Co-60 point source (close geometry)

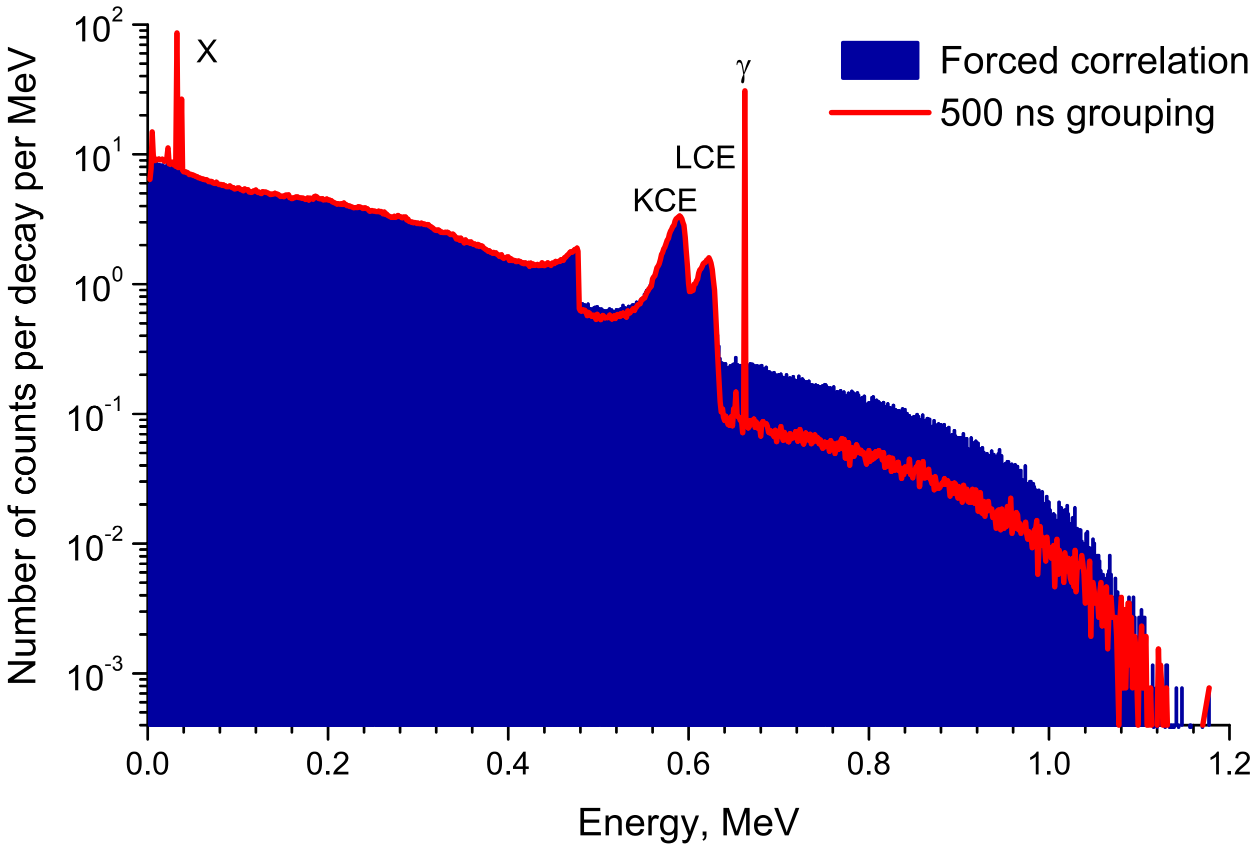


Coaxial 60% HPGe with Eu-152 point source (close geometry)

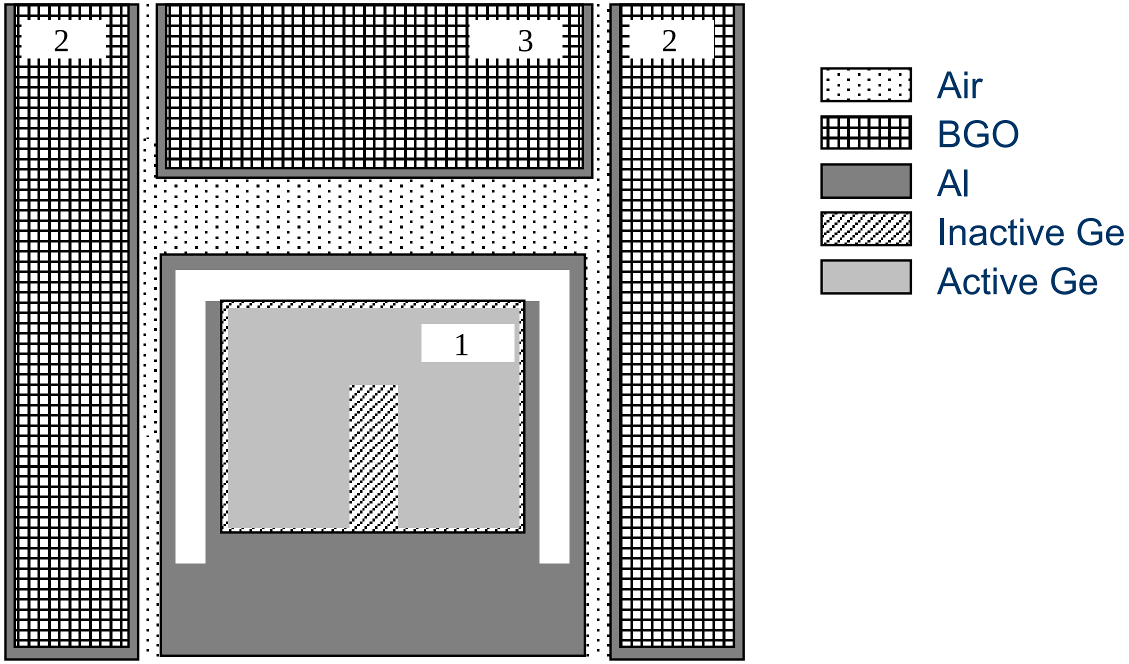


Planar LEGe Detector with Cs-137 point source

(∅16×10 mm, Inactive Ge = 0.3 μm, Be window = 0.005 in.)



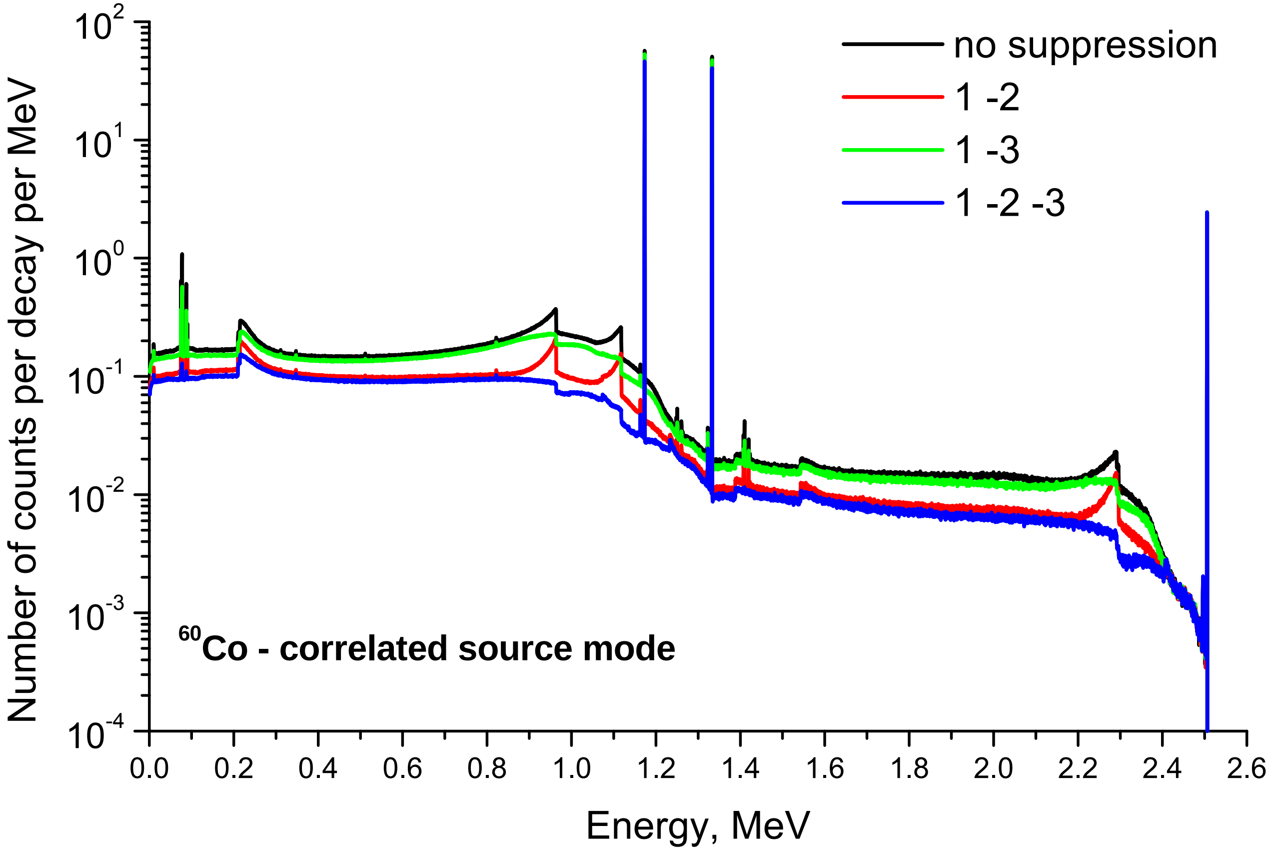
Compton Suppression Spectrometer based on coaxial 60% HPGe and BGO detectors



Analyzing detector: HPGe with relative efficiency 60%, crystal - ∅74×53 mm, inactive germanium – 0.7 mm, rear contact - ∅10×36 mm, crystal cladding – 1 mm of Al.

Guard detectors: annular and plug BGO scintillators with 1.5 mm aluminum coating and thickness 3 and 4 cm respectively.

Compton Suppression Spectrometer with Co-60 point source

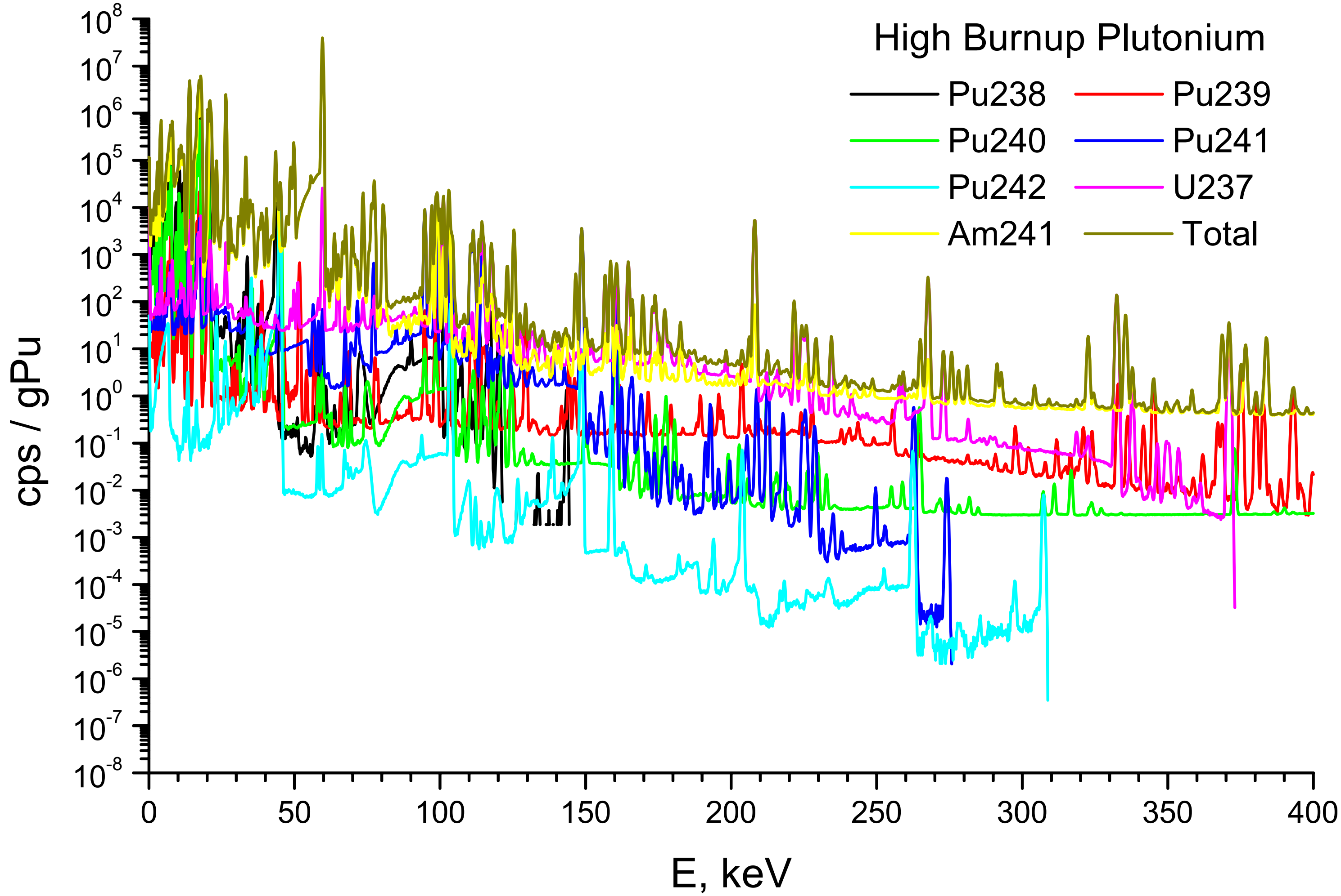


Compton Suppression Spectrometer: coincidence summing corrections calculations*

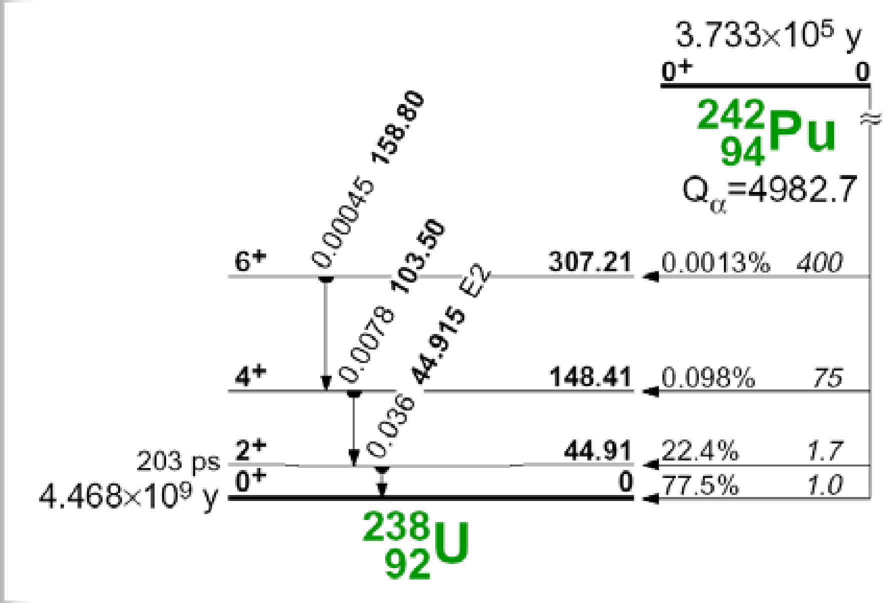
Decay branch	E_γ, keV	Compton Suppression Spectrometer CFs			
		no suppression	plug	annular	plug and annular
^{60}Co→^{60}Ni	1173.25	1.300	1.372	1.511	1.595
	1332.52	1.310	1.392	1.536	1.634
^{152}Eu→^{152}Sm	121.78	1.404	1.537	1.732	1.897
	244.70	1.601	1.932	2.290	2.905
	443.97	1.514	1.730	1.985	2.312
	867.37	1.743	2.562	3.716	7.614
	964.08	1.248	1.422	1.535	1.844
	1085.87	0.889	0.902	0.913	0.926
	1112.07	1.136	1.284	1.376	1.639
	1408.01	1.185	1.344	1.403	1.678
^{152}Eu→^{152}Gd	344.28	1.259	1.335	1.450	1.535
	411.12	1.758	2.269	3.140	4.493
	778.90	1.413	1.696	2.189	2.910

* A.N. Berlizov, V.V. Tryshyn, **A Monte Carlo approach to true-coincidence summing correction factor calculation for gamma-ray spectrometry applications**, Journal of Radioanalytical and Nuclear Chemistry, Vol.264, No.1 (2005) 169-174.

γ-γ coincidence technique for the direct measurement of ^{242}Pu: applicability study



Decay properties of ^{242}Pu



Possible double coincidences:

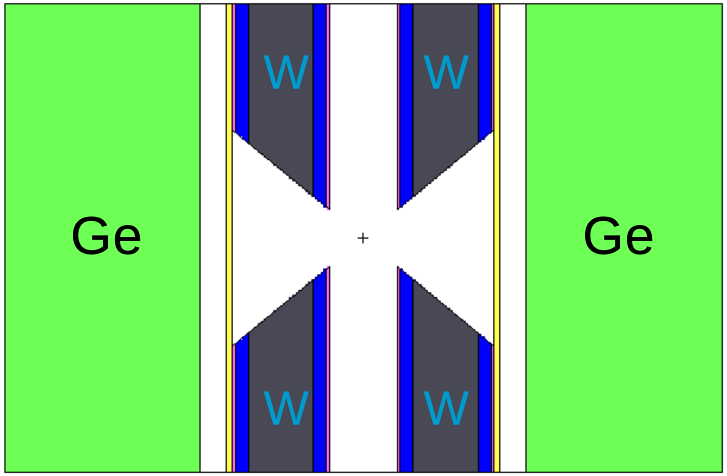
44.9 keV – 103.5 keV
44.9 keV – 158.8 keV
103.5 keV – 158.8 keV

most appropriate

Reasons:

1. Lower energy of 44.9 keV photons will result in higher self-attenuation.
2. Higher intensity of 44.9 keV photons will produce higher background of accidental coincidences.

Measurement setup model



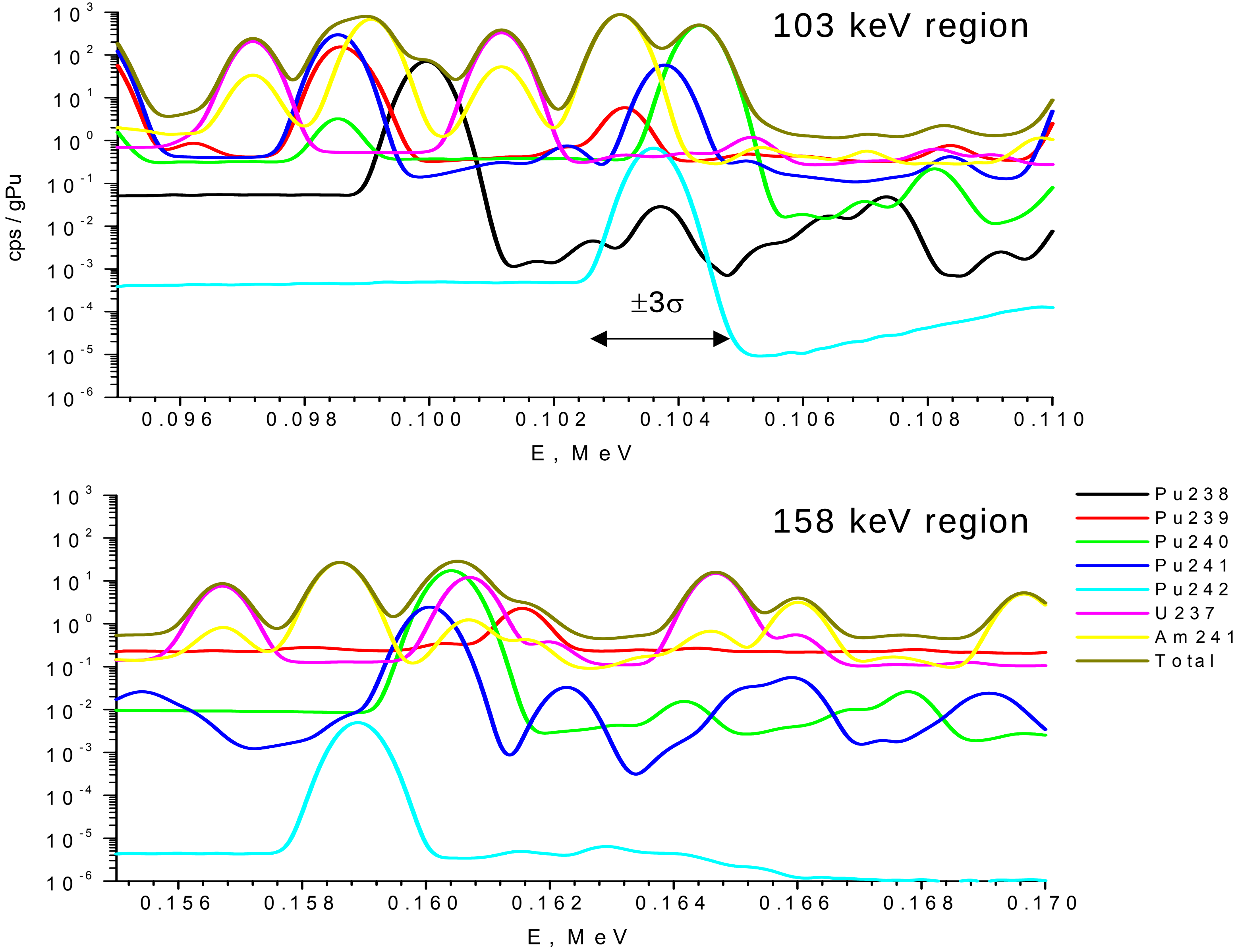
Geometry:

- Detectors: planar HPGe (S=1000 mm^2, d=15 mm);
- Input windows: Al (0.5 mm);
- Collimators: W (5 mm) lined with Cd (1 mm) and Cu (0.2 mm);
- Source: point

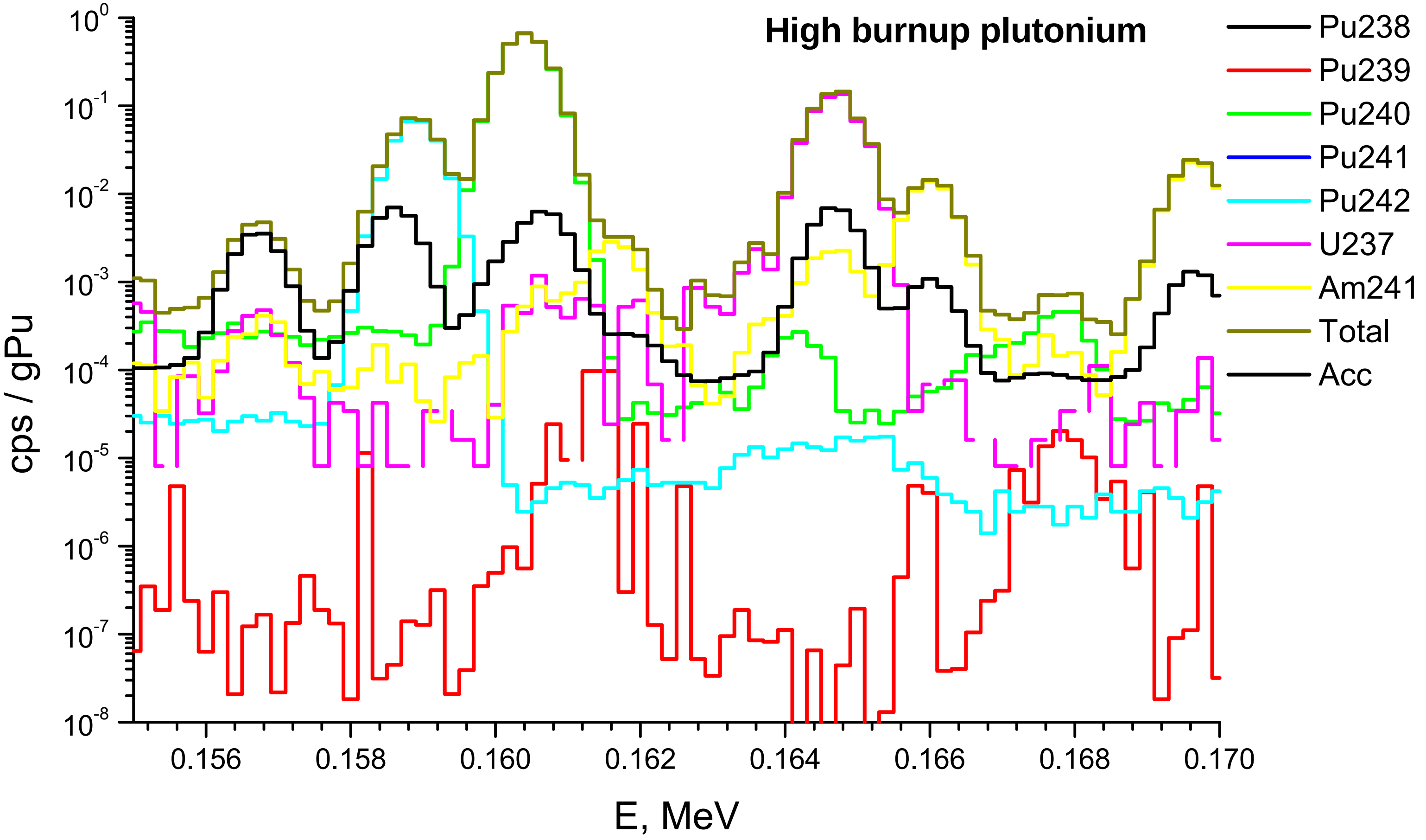
Other parameters:

- FWHM=a+b*E$^{1/2}$, FWHM(5.9 keV)=300 eV, FWHM(122 keV)=600 eV.
- LBU Pu: 0.0109% ^{238}Pu, 93.54% ^{239}Pu, 6.292% ^{240}Pu, 0.1149% ^{241}Pu, 0.0385% ^{242}Pu, 0.201% ^{241}Am (Pu-2000 Sample M).
- HBU Pu: 1.303% ^{238}Pu, 64.99% ^{239}Pu, 24.02% ^{240}Pu, 5.041% ^{241}Pu, 4.642% ^{242}Pu, 4.95% ^{241}Am (Pu-2000 Sample N).

Direct spectra: ROIs



Results: coincidence spectrum



Summary

- A standard MCNP code was extended to allow carrying out calculations with a radiation source emitting correlated nuclear particles.
- A new version of the code, MCNP-CP, performs statistical simulation of processes accompanying radioactive decay of a specified radionuclide, yielding characteristics of emitted correlated nuclear particles, which are then transported through the problem geometry.
- MCNP-CP presents a powerful tool for predicting responses and performance characteristics of conventional single detector as well as advanced multi-detector γ- and β-spectrometry systems.

Thank you for your attention !