Monte Carlo calculation of detector efficiency
GESPECOR and GEANT

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ICRM Gamma WG Meeting Paris Nov. 2006
M. C. Simulations of detector efficiencies

GESPECOR and GEANT 3.21
- 2 sets of results:
  - first set: peak efficiency defined as in experimental work
    (1/10 from the peak height: 96.82 % from Gaussian)
  - second set: ideal peak efficiency (the complete Gaussian)

GESPECOR
- User friendly MC software for solving problems in gamma ray spectrometry with Ge detectors:
  - self-attenuation
  - coincidence summing
  - peak and total efficiency
Peak efficiency definition

- in measurement: based on a region of interest from the peak, e.g. between 1/10 from the peak height (for a Guassian shape, 96.82% from the ideal peak)
- in simulations peak width is not normally reproduced – it depends on charge production and collection etc. Possible to apply a Gaussian spread of the energy deposited in the sensitive volume of the detector, assuming that the peak has a Gaussian shape or simply to take 0.9682 from the ideal efficiency.
- possible practical definitions in simulations based on:
  - interactions in the sensitive volume without any energy lost outside the sensitive volume
  - the number of counts in a suitably defined energy bin
- important to have a consistent use of the definition of the peak, especially when coincidence summing effects are present

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Small angle scattering in the source and the other media problems if an energy bin is used:

- at low energy, weak dependence of scattered photon energy on angle

  e.g. 45 keV: all cases with scattering angle <30° have E>44.5 keV

⇒ Peak efficiency defined using an energy bin might depend on bin width (small angle scattering; rounding errors)
⇒ it might be also influenced by the environment of the measurement, not only by the source, detector and media in between

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Geometry 2 and 3 Spectrum at 45 keV

Geometry 2 (normalized)

Geometry 3

K$_\beta$ escape peak

Number of counts

Energy (keV)

10^5

10^4

10^3

10^2

10^1

1

0

0.01

0.02

0.03

0.04

0.05

45 keV
GESPECTOR: physics

Photon cross sections:
- for each material 100 points between 1.9 keV and 4 MeV; in addition, values before and after each X-Ray absorption edge, on the basis of XCOM
- log-log interpolation
- very good accord with XCOM (also in the close vicinity of absorption edges)

Electron processes:
- multiple scattering (Moliere, third function included), or faster semiempirical method
- bremsstrahlung: fast algorithm, sampling using Walker algorithm
- energy loss fluctuations neglected
- delta electron production neglected
- energy cut: 10 keV

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GESPECOR – variance reduction

- Peak and total efficiency evaluated separately:
  - peak efficiency: photon history stopped when energy lost outside the sensitive volume of the detector
  - materials between the point of emission and the sensitive volume of the detector: attenuating media
  - emission from source: focalized towards the detector
  - total efficiency: photon history stopped at the first interaction in the sensitive volume of the detector
- Always force the first interaction in the detector
- Whenever possible use mean values instead of random sampling (e.g. use probability of the emission of groups of photons instead of random simulation of decay cascades in coincidence summing computations)
- Use efficient sampling (Walker, interpolation)
Intercomparison results

Comparison between our results obtained with GESPECOR and with GEANT:
- in geometry 1 reasonable agreement
- in geometry 2 and 3 higher discrepancies, especially at low energies
Agreement of the results for geometry 1 implies that cross sections are in accord?
- no, in geometry 1 at low energy the detector is practically an „infinitely thick“ detector, irrespective to the exact values of the cross sections.
- in fact, important differences between XCOM and GEANT cross sections, especially in photoelectric cross section (XCOM – from NIST, Berger and Hubbell)
Peak Efficiency

GESPECOR versus GEANT

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Differences in photon cross sections in Ge

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Differences in photon cross sections in Al and H2O

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XCOM versus GEANT

Energy (MeV)

% Difference

Al Photoeffect
H2O Photoeffect

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Effect of the differences in cross sections in the case of geometry 1:
- at 45 keV, peak efficiency is changed by 0.08% and total efficiency is changed by 0.07% if artificial Ge density equal to 6 g/cm$^3$ (instead of 5.323) is used in GEANT calculations.

Effect of differences in cross sections in the case of other geometries:
- at 45 keV, if in GEANT the dead layer density is changed from 5.323 g/cm$^3$ to 5.565 and the Al density is changed from 2.7 g/cm$^3$ to 2.828, the XCOM and GEANT 3.21 cross sections become equal:
  => change in peak efficiency $-12.6\%$ (G2)
  => change in total efficiency $-12.2\%$ (G2)
- at 45 keV if in GESPECOR the cross sections are modified artificially to be equal to the GEANT cross sections, the differences between GESPECOR and GEANT decrease to 0.5% (G2) and 1.2% (G3) (Ge X-Ray escape excluded).
At low energy photon attenuation in the media between the emission point and the sensitive volume of the detector are most important.

⇒ dependence on the photon cross sections (especially for photoeffect)

⇒ Which cross sections are the best?

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Effect of the low energy cut-off:
- in GESPECOR 1.9 keV for photons, 10 keV for electrons
- in GEANT 3.21 10 keV for photons, 10 keV for electrons

Computations with GEANT also with 15 and 20 keV low energy cut-off

⇒ small change in peak efficiency, practically no change in total efficiency
Is the 10 keV energy cut-off of no importance?

Ge K X-Rays: \( K_{\alpha 2} \) 9.85543 (51.49%),

\( K_{\alpha 1} \) 9.88653 (100%), \( K_{\beta 3} \) 10.9781 \( K_{\beta 1} \) 10.9822

\( K_{\beta 3''} \) 11.0748 (22.37), \( K_{\beta 2} \) 11.101 (0.49%)

=> 6.63 times higher probability of X Rays with \( E < 10 \) keV than with \( E > 10 \) keV

If in GESPECOR the simulation of Ge X-Rays is prohibited, the discrepancy in geometry 1 at low energies between GESPECOR and GEANT is much reduced
Geometry 1 Spectrum at 45 keV

- Low energy cut 10 keV
- Low energy cut 12 keV

Kβ escape peak

Number of counts

Energy (keV)
Computing times: ACER Notebook, Pentium M Centrino 1.4 GHz

<table>
<thead>
<tr>
<th>Geometry</th>
<th>GESPECOR</th>
<th>GEANT</th>
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<tbody>
<tr>
<td>Geometry 1</td>
<td>Peak efficiency: 3 min</td>
<td>1100 min</td>
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<tr>
<td></td>
<td>Total efficiency: 3 min</td>
<td>3 min</td>
</tr>
<tr>
<td>Geometry 2</td>
<td>Peak efficiency: 4 min</td>
<td>2150 min</td>
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<td>Total efficiency: 15 min</td>
<td>15 min</td>
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<tr>
<td>Geometry 3</td>
<td>Peak efficiency: 8 min</td>
<td>17000 min</td>
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<tr>
<td></td>
<td>Total efficiency: 60 min</td>
<td>60 min</td>
</tr>
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Conclusions

Monte Carlo methods are very useful for assisting in gamma ray spectrometry calibration problems
- Good cross sections are required
  - most important: photoelectric cross sections
- Low energy cut should be low enough
- Good knowledge of the details of the media between the source and the active volume of the detector