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Analytic Gamma-Ray Detector Response Function (DRF) Rev. 1

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National Nuclear Security Administration

Objectives

- **Enable fast and accurate computation of gamma-ray detector response to support various applications, including the following:**
  - Detection and identification of smuggled nuclear materials
  - Diagnostic evaluation of terrorist devices containing special nuclear materials (SNM)
  - Material control and accountability
  - Arms control inspections
  - Emergency response following nuclear accidents
  - Environmental surveys
  - Health physics
- **Recurring calculations are all completed in a few seconds or less**
- **Some libraries, such as gamma and neutron scattering, are computed by Monte Carlo methods**

Analytic Approach

- **Interactions are represented by analytic expressions**
  - Nested loops describe sequential events
- **Numerous approximations are applied to enable rapid solution**
  - Probabilities are represented rather than tracking individual interactions
- **Monte Carlo calculations are used in some cases to compile libraries that are used for subsequent interpolation**
  - Gamma-rays and neutrons that scatter into detectors are modeled this way
- **Continuous functions applied to all phenomena**
  - Parameters can be evaluated by standard regression methods
- **Empirical parameters are applied to describe some phenomena**
  - Resolution and energy calibration
  - Nonlinearities (property of crystal and photomultiplier for scintillators)
- **The DRF and radiation transport calculations are tightly coupled**
  - Ray-trace and discrete ordinates are combined by the DRF

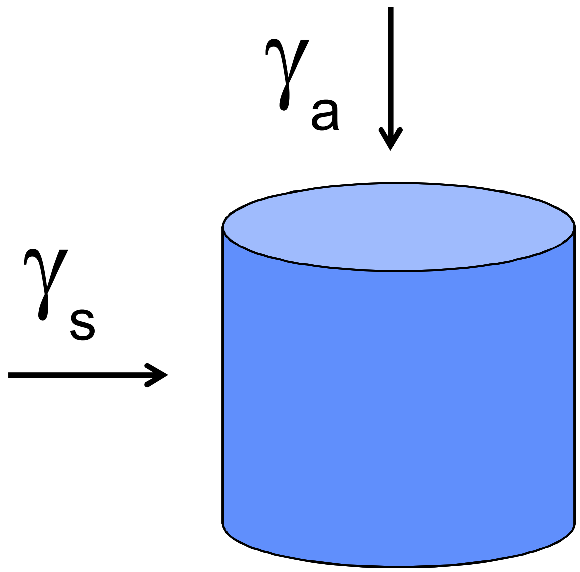
Chemical Formulas Dictate Interactions

content of file “DetectorData.gadras” below

Number	Name	Formula	Density	Resolution
1	BGO	Bi4Ge3O12	7.125	16
2	CsI	CsI	4.51	8
3	HPGe	Ge	5.33	0.25
4	HgI	HgI2	6.4	1
5	NaI	NaI	3.667	7
6	PVT	C1H1.104	1.03	20
7	Si	Si	2.33	0.3
8	CZT	Cd0.96Zn0.04Te	5.78	2
9	CdTe	CdTe	5.85	3
10	LaCl3	LaCl3	3.84	4
11	LaBr3	LaBr3	5.06	2.5
12	CdWO4	CdWO4	7.90	14
13	Xe	Xe	0.1	4
14	CaF2	CaF2	3.18	10
15	CLYC(nat)	Cs2LiYCl6	3.31	4
16	CLYC(95%)	Cs2LiYCl6	3.31	4
17	SrI2	SrI2	4.59	3
18	YAP	YAlO3	5.37	6
19	PFCBBr	C8H3OBr4	3.6	20
20	BaFBr:Eu	BaFBr	4.96	20

Path Length for First Interaction

- **How to describe the detector shape?**
  - The profile is flat for photons striking a cylindrical detector along the axis
  - The profile is circular if irradiated from the side



Path Length for First Interaction

- **How to describe the detector shape?**
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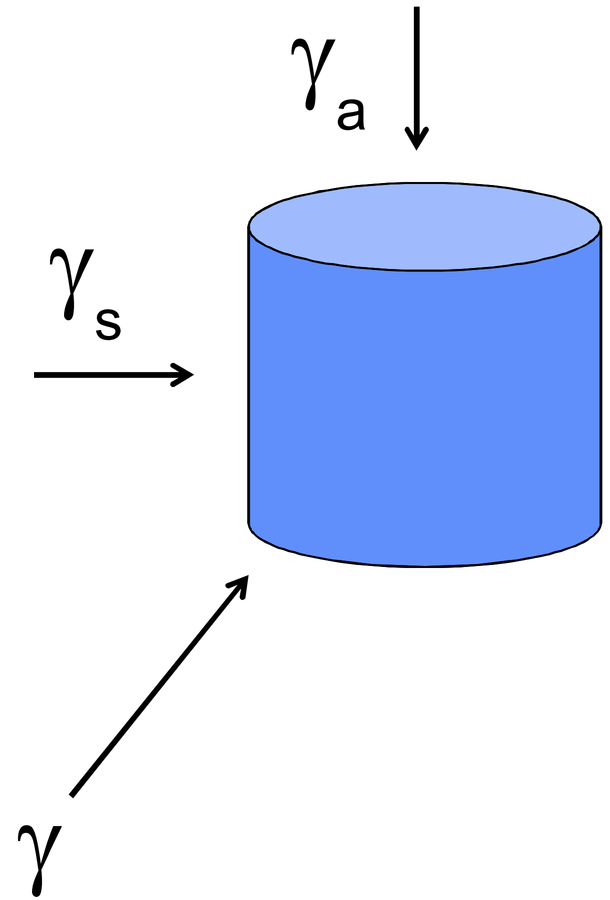
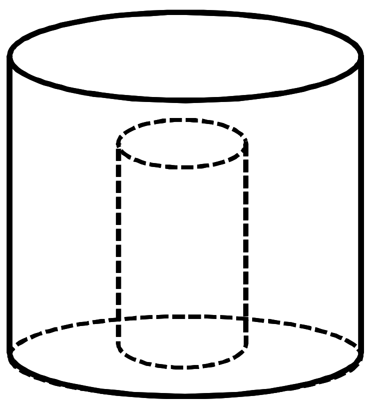


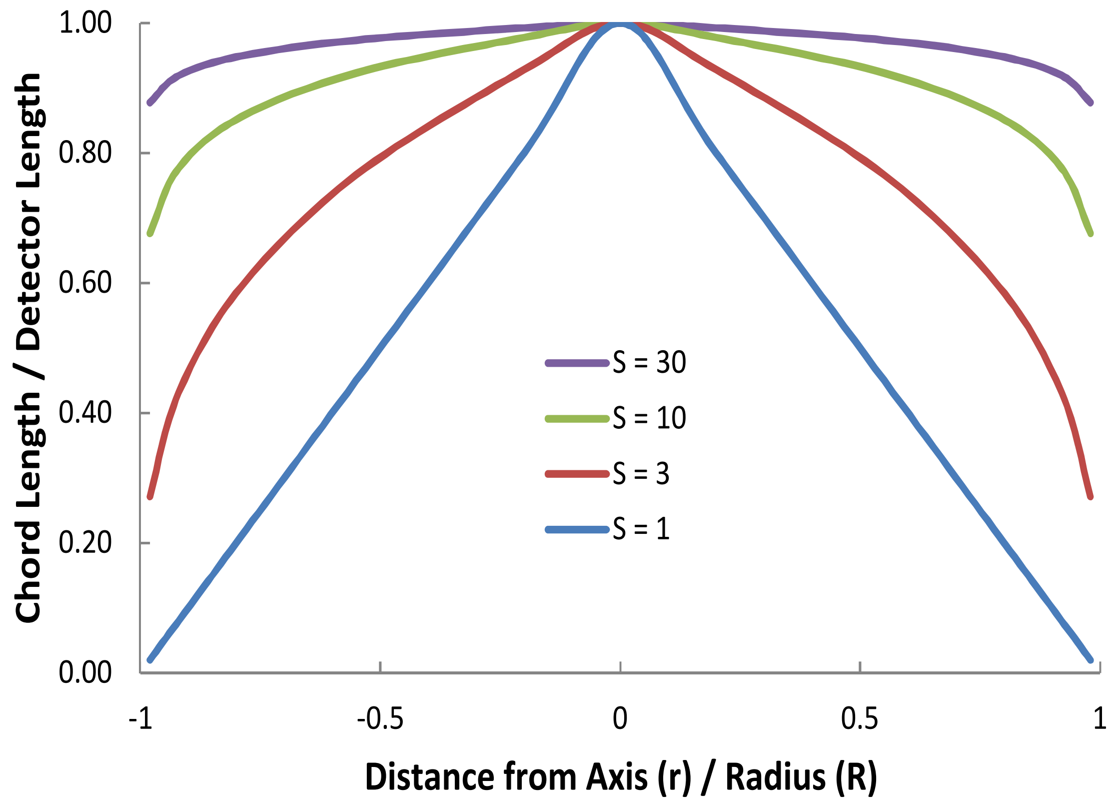
- **What about HPGe detectors with cavities or unusual angles of incidence?**



Path Length for First Interaction

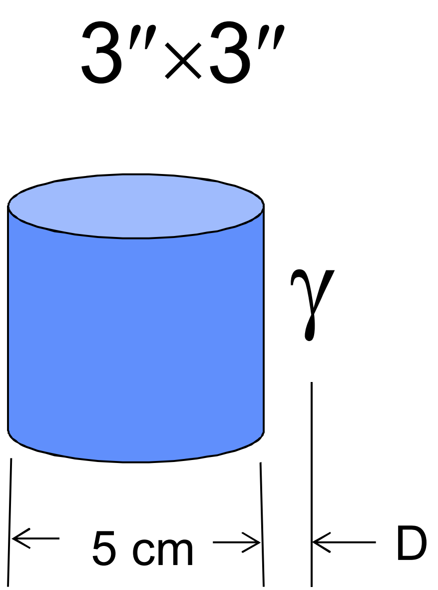
- **A continuous function is used to describe a variety of shapes in terms of a shape parameter S**
  - S > 20 describes flat profile
  - S = 3 for circular profile

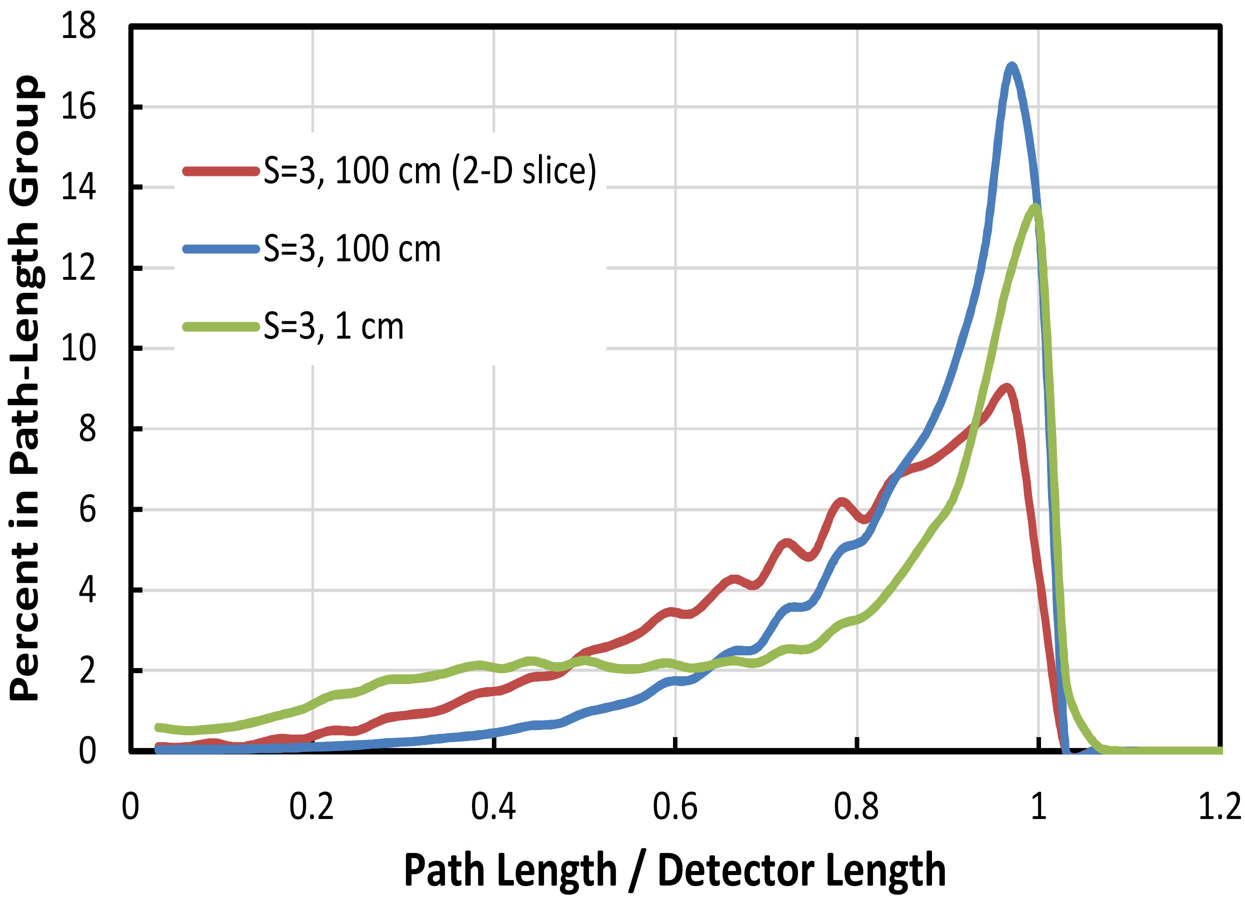
$$L = \left(1 - \frac{r}{R}\right)^{\left(\frac{1}{S}\right)}$$



Path Length Distributions can be Interesting

- **The same shape parameter (S) applies regardless of distance, but geometric effects alter the path length distribution**

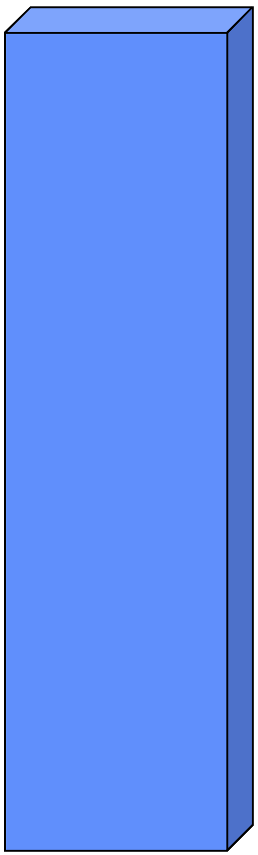


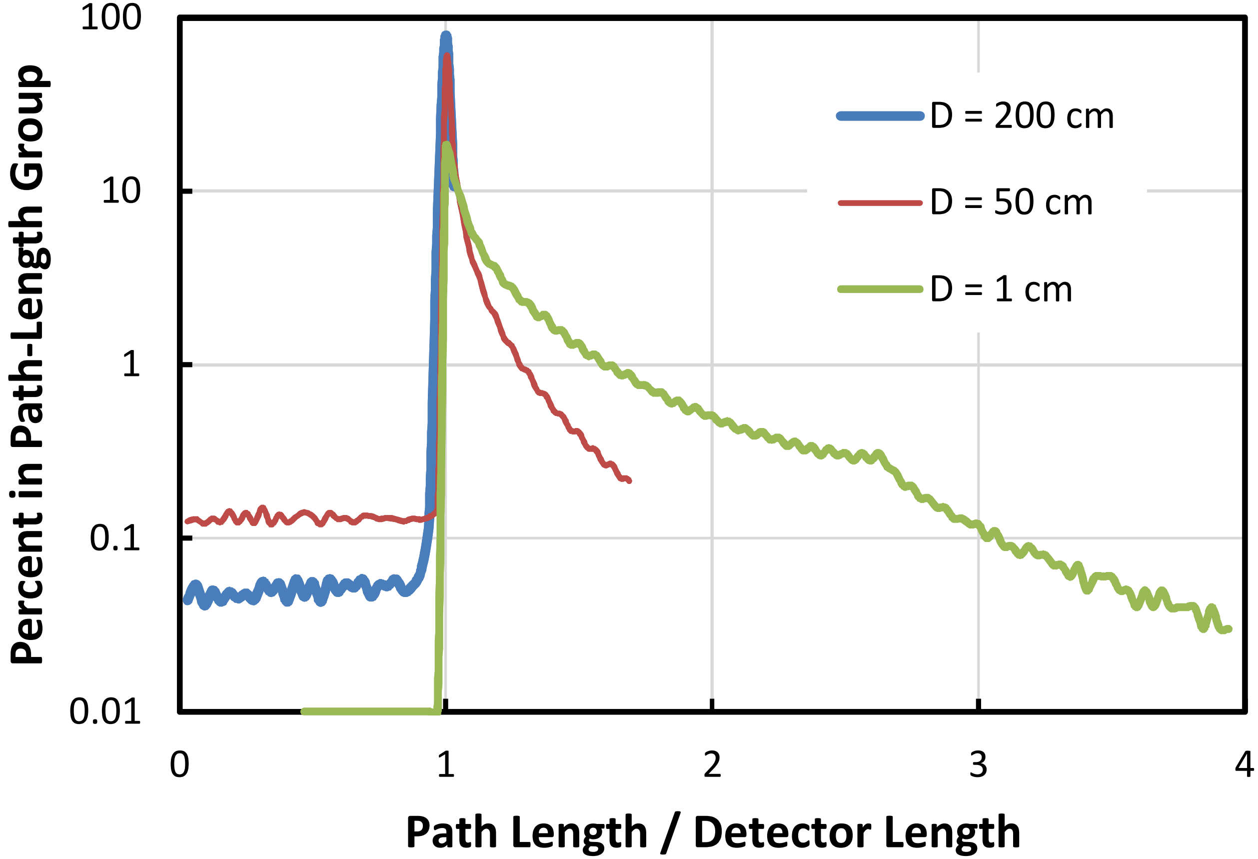


Path Length Distributions can be Interesting

- **Portal detectors are very thin relative to height and width**

1.5″×10″×60″





Interactions within the Detector

- **The initial interaction leads to three possible events**
  - **Photoelectric absorption**
    - Photon energy is imparted to a recoil electron (leaving an inner-shell vacancy)
    - Most interactions deposit full energy in detector, except:
      - Leakage of recoil electron before full energy absorption
      - The escape of K-shell and L-shell x-rays
  - **Pair production**
    - An electron and a positron are created
      - The positron annihilates with an electron, creating two 511-keV gamma rays departing in opposite directions
      - Each 511-keV gamma ray may escape, scatter or be fully absorbed
  - **Compton scatter (most probable event for E(γ) >200 keV)**
    - The energy of the incident photon is shared by the recoil electron and the scattered photon
      - The energy of the scattered photon is correlated with the scattering angle
      - Most of the recoil electrons are fully absorbed (except as noted above)
      - Most of the scattered photons generally scatter again or escape

How to Describe these Interactions?

- In the words of my colleague Jon Bradley:

Tell me what happens without using the words "it depends"

Photoelectric | Compton

$$\gamma \longrightarrow \begin{matrix} \text{X-ray} \\ + \\ {}^{-}e_a \end{matrix} \;\text{or}\; \begin{matrix} \gamma_a \\ + \\ {}^{-}e_a \end{matrix} \longrightarrow \begin{matrix} \text{X-ray} \\ + \\ {}^{-}e_b \end{matrix} \;\text{or}\; \begin{matrix} \gamma_b \\ + \\ {}^{-}e_b \end{matrix} \longrightarrow \ldots$$

Any or all of the photons and electrons can escape

- Analytic models require algorithms to describe each interaction, and these algorithms are nested into loops to create probability distributions
- Analytic models can be instructive because terms can be turned on and off to examine the impact of various phenomena

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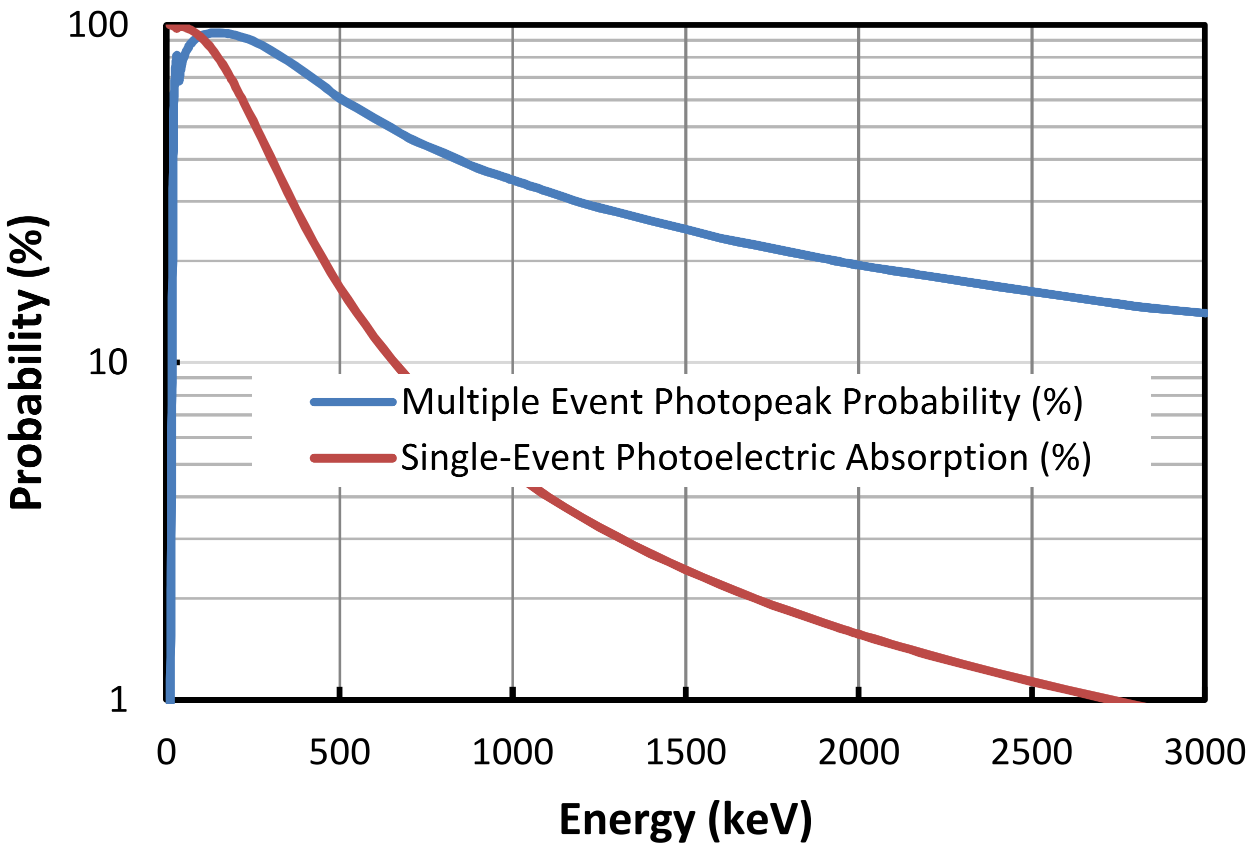
Photoelectric Absorption (3″×3″ NaI)

- **Photopeaks derived from single-event photoelectric absorptions are only probable at low energy**
  - Compton scattering followed by photoelectric absorption of lower energy photons dominate above about 200 keV



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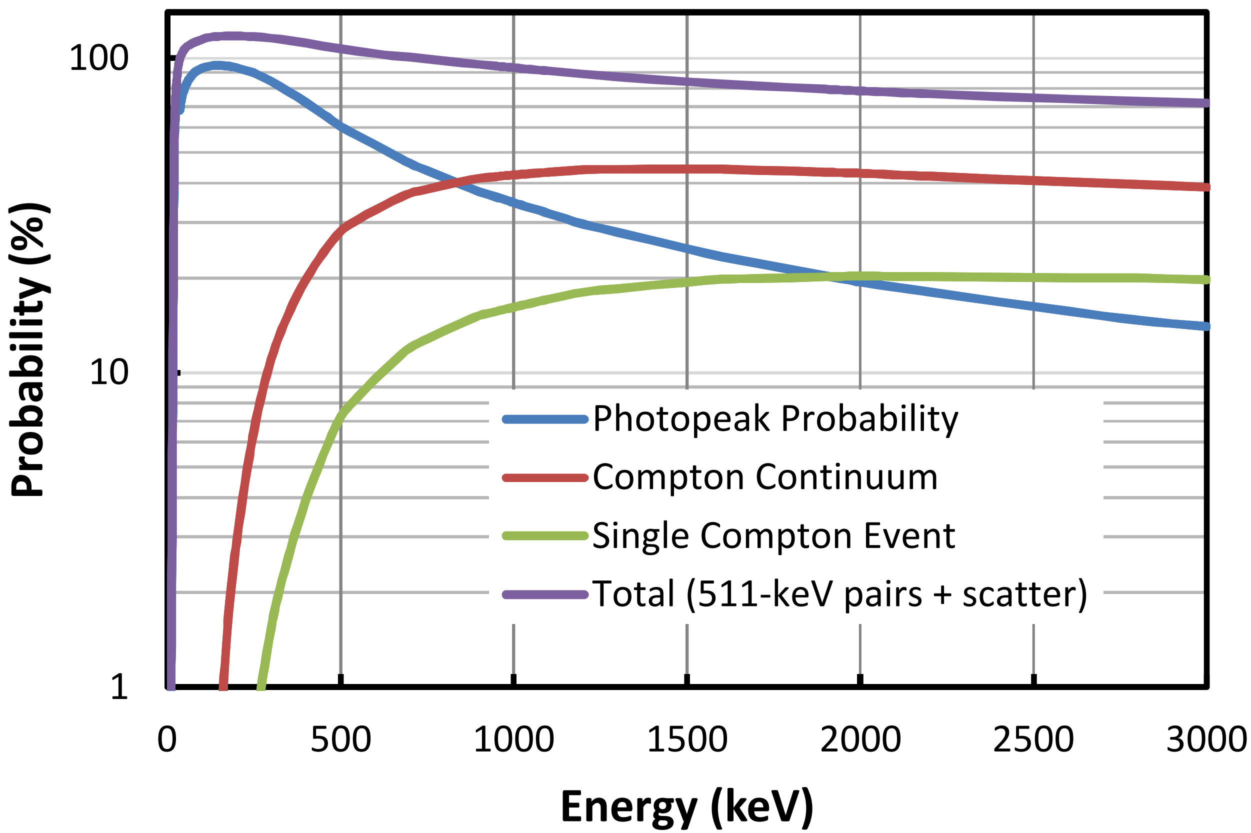
All Interactions (3″×3″ NaI)

- **Compton continuum dominates above about 1000 keV**
  - Multiple Compton scatter represents ~50% of continuum in NaI & HPGe
  - Total efficiency can exceed 100% when photons that scatter into the detector are included



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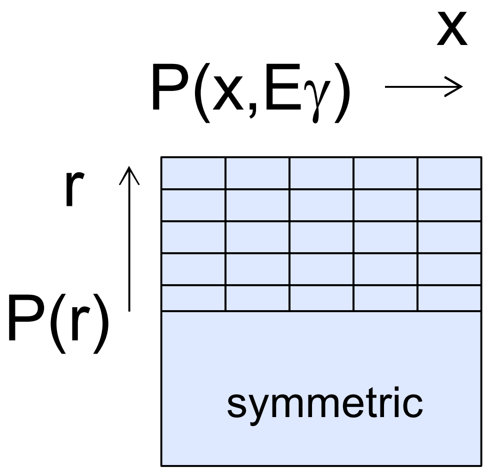
Compton Scatter out of the Detector

- **First scatter event**
  - The relative depth of first scatter events is a function of the gamma-ray energy and the detector material
  - The probability of a volume element as a function of displacement relative to the detector axis is defined by the detector shape and distance from the source
  - The probability of scattering is computed as a function of θ, $E\gamma$
  - The escape probability is computed as a function of $E\gamma'$, x, r, θ and φ

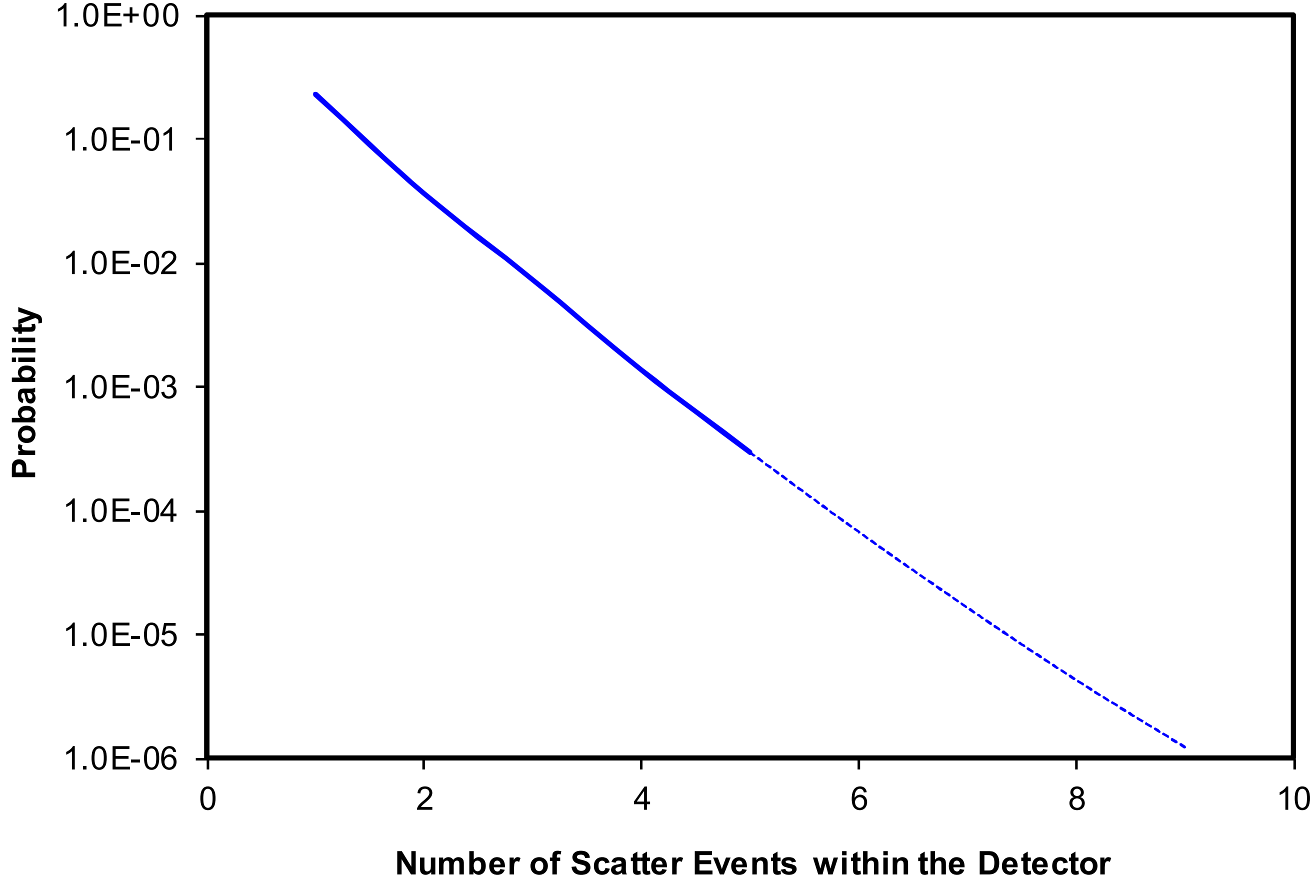


- **Second scatter events**
  - The probability as a function of depth and radial displacements for second scatter events don't change much relative to first scatter events. Therefore, the same spatial profiles can be applied
  - The angular correlations of between first and second scatter events are important

Compton Scatter Out of the Detector

- **Third scatter events**
  - After two scatter events, the distributions can be approximated as “photon soup”, where the angular distributions are isotropic
  - Angles don’t matter any more, which speeds the calculations
  - The same depth and radial concentration distributions can be applied
- **Higher-order scatter events**
  - More of the same
- **Electrons can leak from the detector surfaces**
  - Electrons may leak following either photoelectric absorption or Compton scatter
  - The probability of an individual electron leaking from a surface before depositing the full energy is not very high, but the probability of one of many electrons leaking is significant
  - Electron leakage introduces a continuum that is forward biased toward the full electron energy (unless the detector is very small)

Multiple Compton Scatter for 2″×2″ PVT

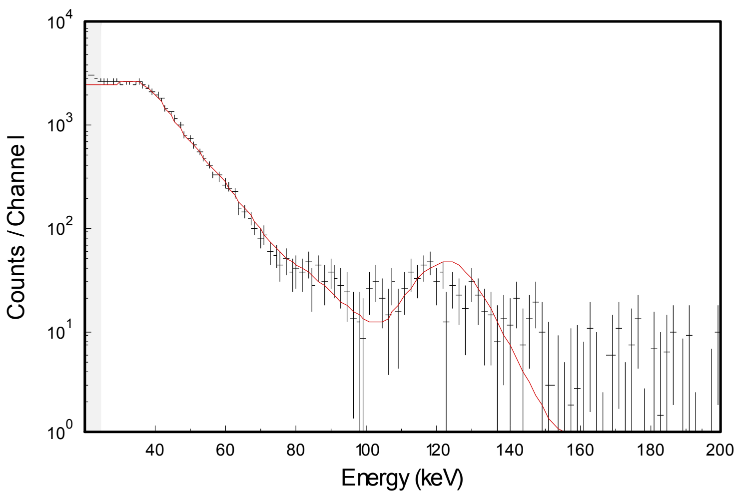


The Compton scatter subroutine tracks five scatter events explicitly and extrapolates probabilities to higher-order scatter events

Computed vs. Measured Spectra for 2"× 2" PVT

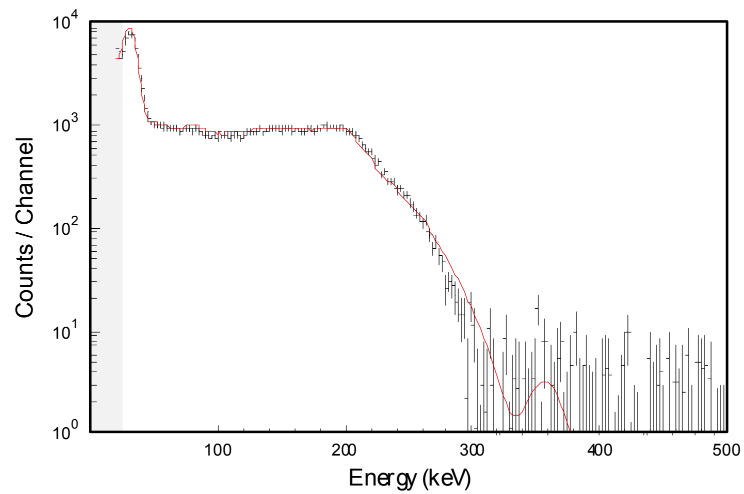
Co-57 @ 20 cm

live-time(s) = 600.00
chi-square = 1.02



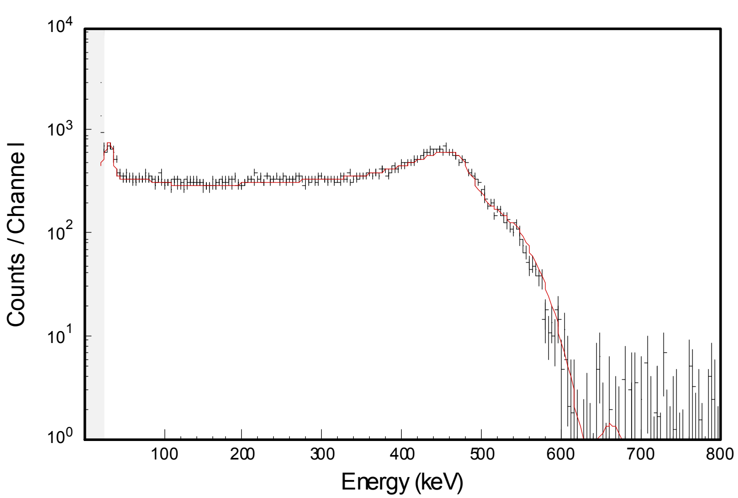
Ba-133 @ 20 cm

live-time(s) = 400.00
chi-square = 1.26



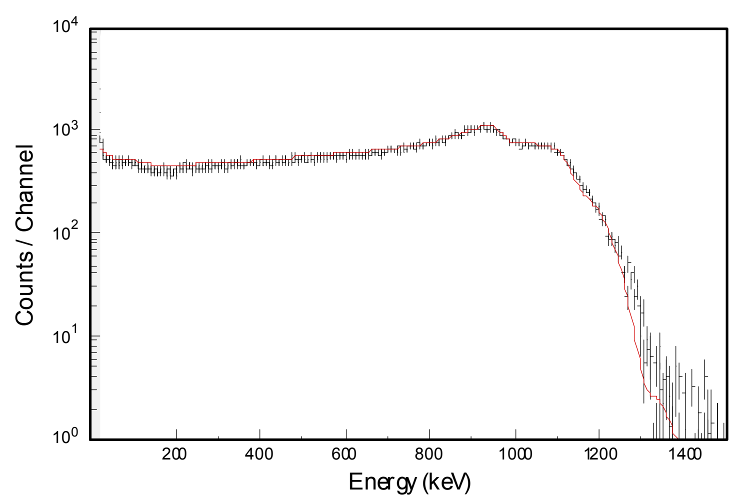
Cs-137 @ 20 cm

live-time(s) = 400.00
chi-square = 0.97

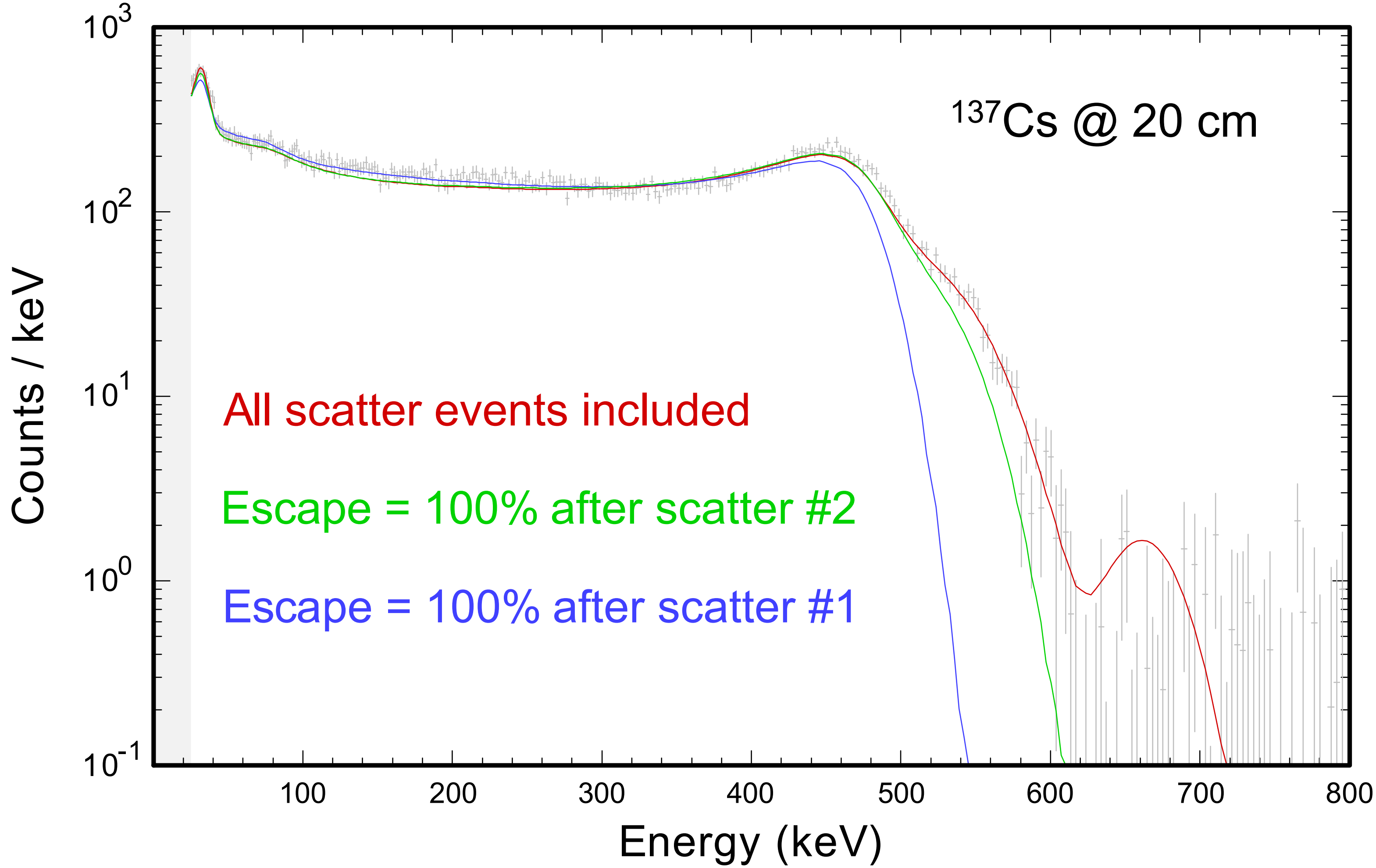


Co-60 @ 20 cm

live-time(s) = 400.00
chi-square = 1.82



Change in Spectrum for 2"× 2" PVT with Number of Compton Scatter Events



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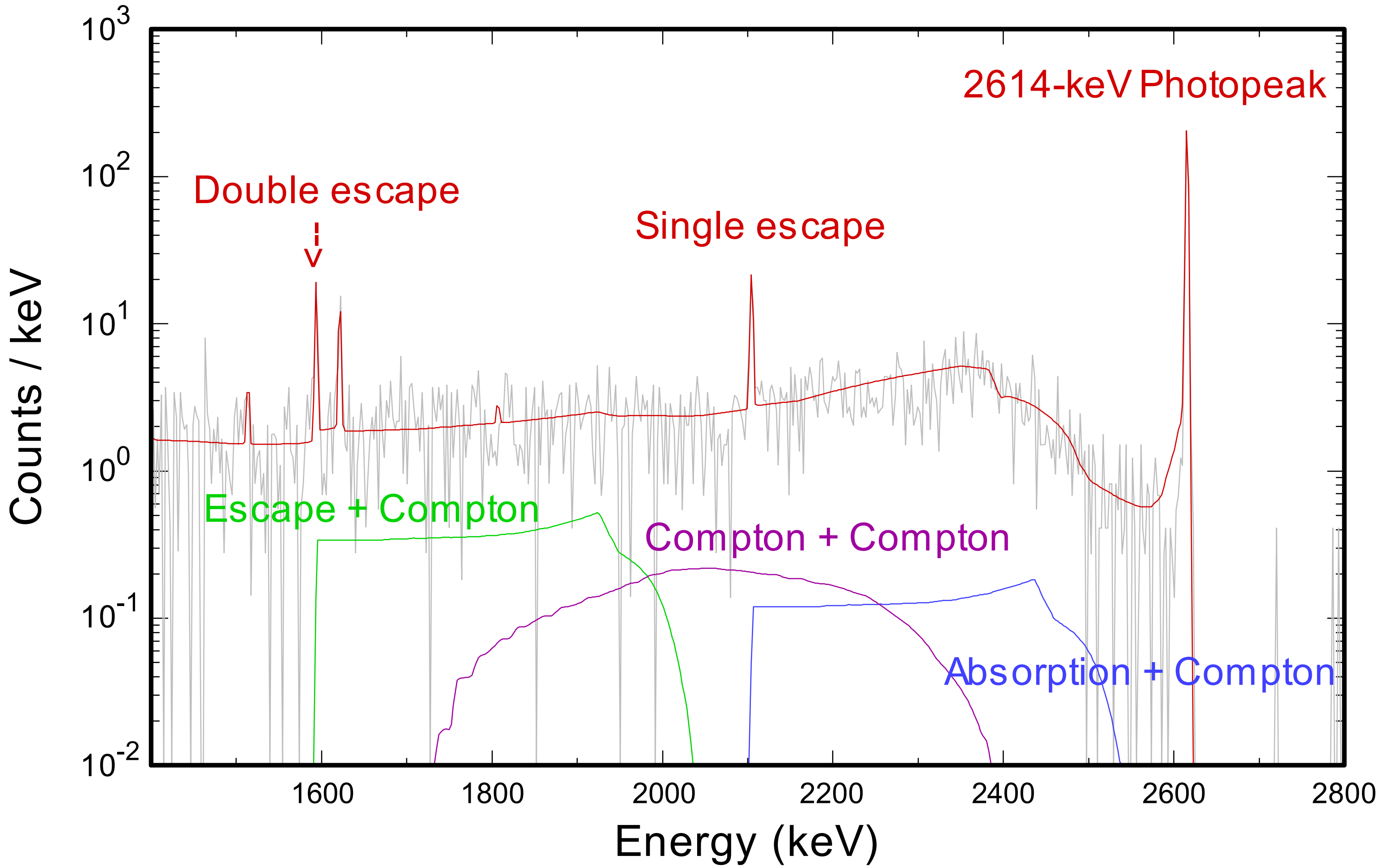
Pair Production

- **An electron-positron pair can be created for gamma rays exceeding twice the rest mass of an electron (1022 keV)**
  - The incident gamma-ray is converted to an electron-positron pair
  - Excess kinetic energy shared by the pair is absorbed in detector
    - The deposited energy is at least $E\gamma$-1022 keV
  - The positron annihilates with an electron, creating two 511-keV photons that are emitted in opposite directions
- **Possible events following pair production**

First 511-keV γ	Second 511-keV γ	Outcome
Escape	Escape	Double escape peak
Escape	Complete absorption	Single escape peak
Escape	Compton scatter / escape	Continuum $E\gamma$-1022 to $E\gamma$-511
Compton scatter / escape	Compton scatter / escape	Continuum $E\gamma$-1022 to $E\gamma$
Complete absorption	Compton scatter / escape	Continuum $E\gamma$-511 to $E\gamma$
Complete absorption	Complete absorption	Adds to full-energy peak

Pair Production and Spectrum Shape

Region in ^{228}Th spectrum associated with 2614-keV gamma from ^{208}Tl daughter



X-Ray Escape from Gamma-Ray Detectors

- Photoelectric absorption is the dominant process in most detectors for photons less than about 200 keV.
- Gamma-ray is completely absorbed by an atom, and a photoelectron is ejected from a bound shell.
- X-rays are emitted when electrons from less tightly bound shells drop into vacancies produced by the photoelectric absorption.
- Some of the x-rays escape, resulting in x-ray escape peaks.
- The energies of x-ray escape peaks equal the difference between the incident gamma-ray energy and the energy of the escaping x-ray.
- Areas of x-ray escape peaks are normally smaller than areas of associated photopeaks, and they may not be resolvable, particularly true for low-resolution detectors.
- Nevertheless, x-ray escape peaks influence gamma-ray spectra.
  - Non-Gaussian peak shapes can be difficult to understand if x-ray escape is neglected.

X-Ray Escape Model

- Fluorescence x-rays only escape if they are generated near the surface
  - Half of the photons are absorbed within 0.01 cm of the surface when an HPGe is exposed to 30 keV photons
- Escape x-ray yields can be estimated by a relatively simple model that only represents the near-surface region, and details concerning the detector dimensions and shape are relatively unimportant
  - Modified in 2014 for leakage through other surfaces (very small detectors)

$$Y_{ij} = \frac{\omega_k W_j f_{ij} \left(\frac{\mu_{K_{ij}}(E_\gamma)}{\mu_T(E_\gamma)} \right) \int e^{-\mu_T(E_\gamma)\rho x} L(E_{ij}, x)\, dx}{\int e^{-\mu_T(E_\gamma)\rho x}\, dx}$$

Y_{ij}	Yield of x-ray *i* emitted by element *j*	$\mu_T(E\gamma)$	Total cross section for incident gamma ray
ω_k	Fluorescence yield of k-shell electron	$\mu_{Kij}(E\gamma)$	Cross section for K-shell fluorescence
W_i	Weight fraction element j	ρ	Density of detector material
f_{ij}	Fraction of emission of x-ray i relative to total x-rays emitted by element *j*	$L(E_{ij},x)$	Average leakage probability for an x-ray of energy E_{ij} following photoelectric absorption at depth x in the detector material

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X-Ray Escape Model (continued)

- It is assumed that all x-rays traveling deeper into the detector are fully absorbed (i.e., $L(E_{ij},x)=0$ for $\theta \geq 90°$)
- The average leakage probability is given by the following equation:

$$L(E_{ij},x) = \frac{\int_0^{89} e^{-\mu_{T_{ij}}\rho\left(\frac{x}{\cos(\theta)}\right)} \frac{dA}{d\theta} d\theta}{\int_0^{180} \frac{dA}{d\theta} d\theta}$$

where *dA/d*θ is the derivative of the surface area of a unit sphere with respect to θ.

- The x-ray leakage probabilities only need to be solved once for a new detector material because the size and the shape of the detector are inconsequential
- The calculation takes a couple seconds

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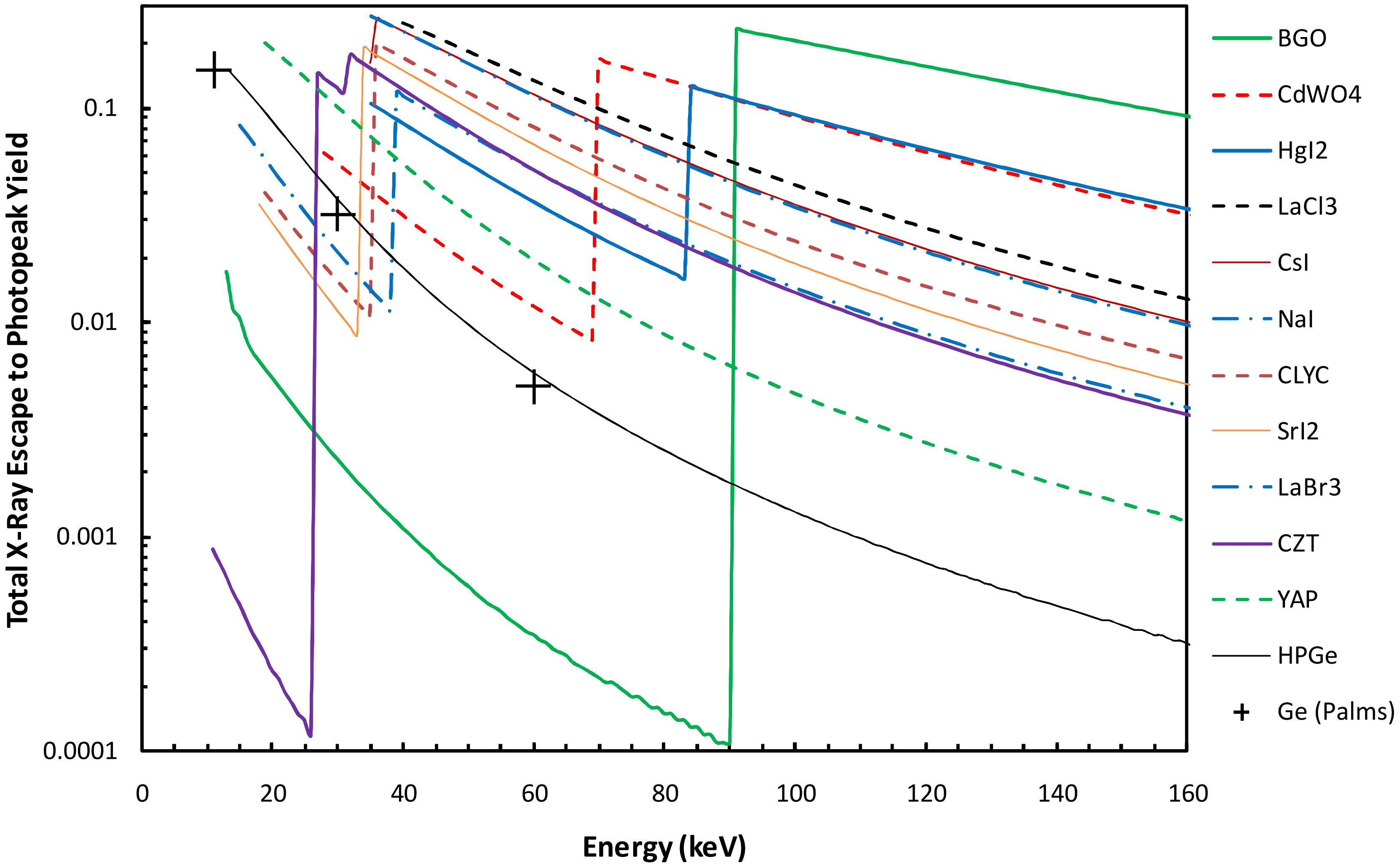
Total Yields for X-Ray Escape Peaks



Computed yields are about 10% greater than published yields (Palms) for HPGe

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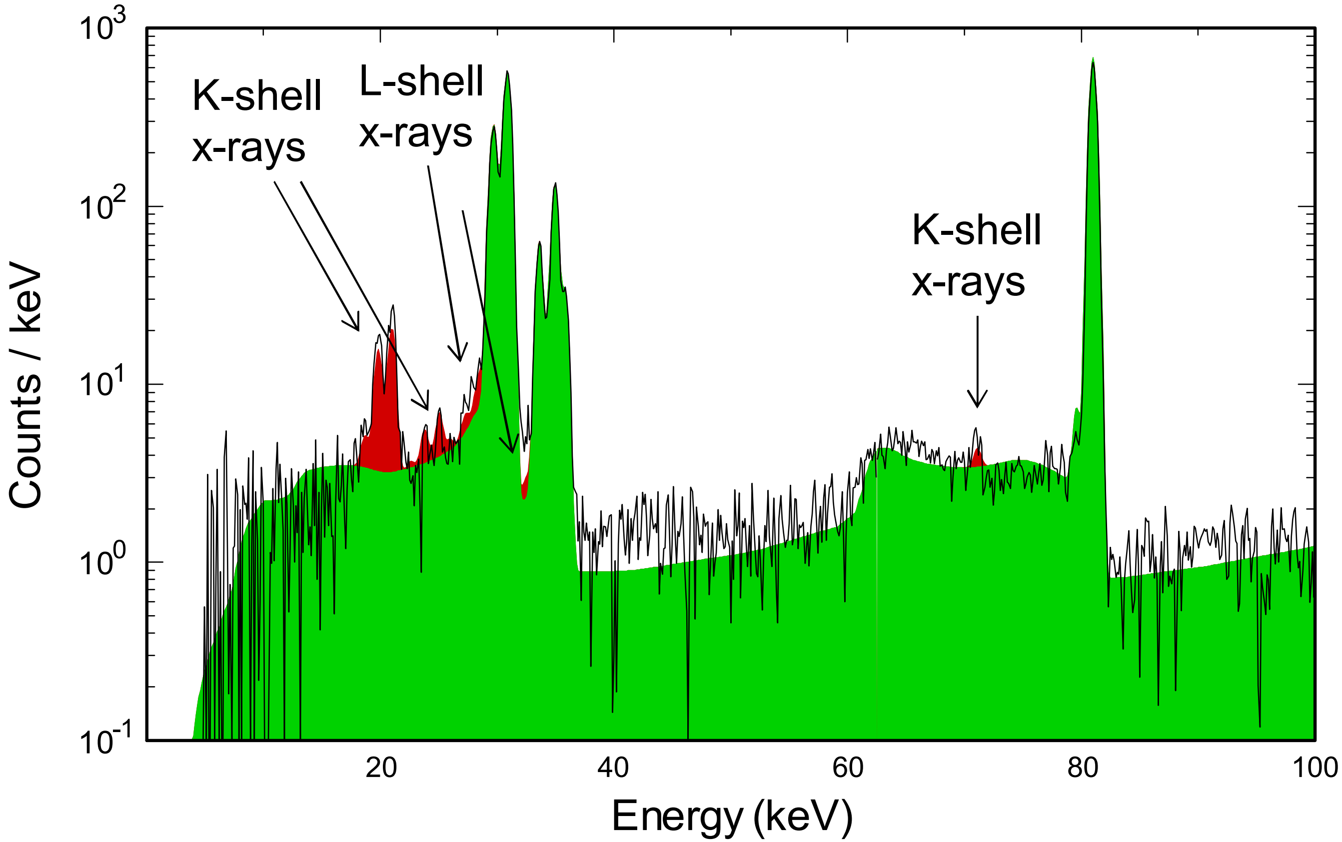
X-Ray Escape Peaks in an HPGe Spectrum



- Spectrum for ^{131}Xe, ^{131m}Xe, ^{135}Xe and ^{133m}Xe measured with a Canberra Falcon 5000
  - Green region shows calculation without x-ray escape peaks (the photopeak intensities are reduced slightly when x-ray escape peaks are included)
  - Red regions show x-ray peaks

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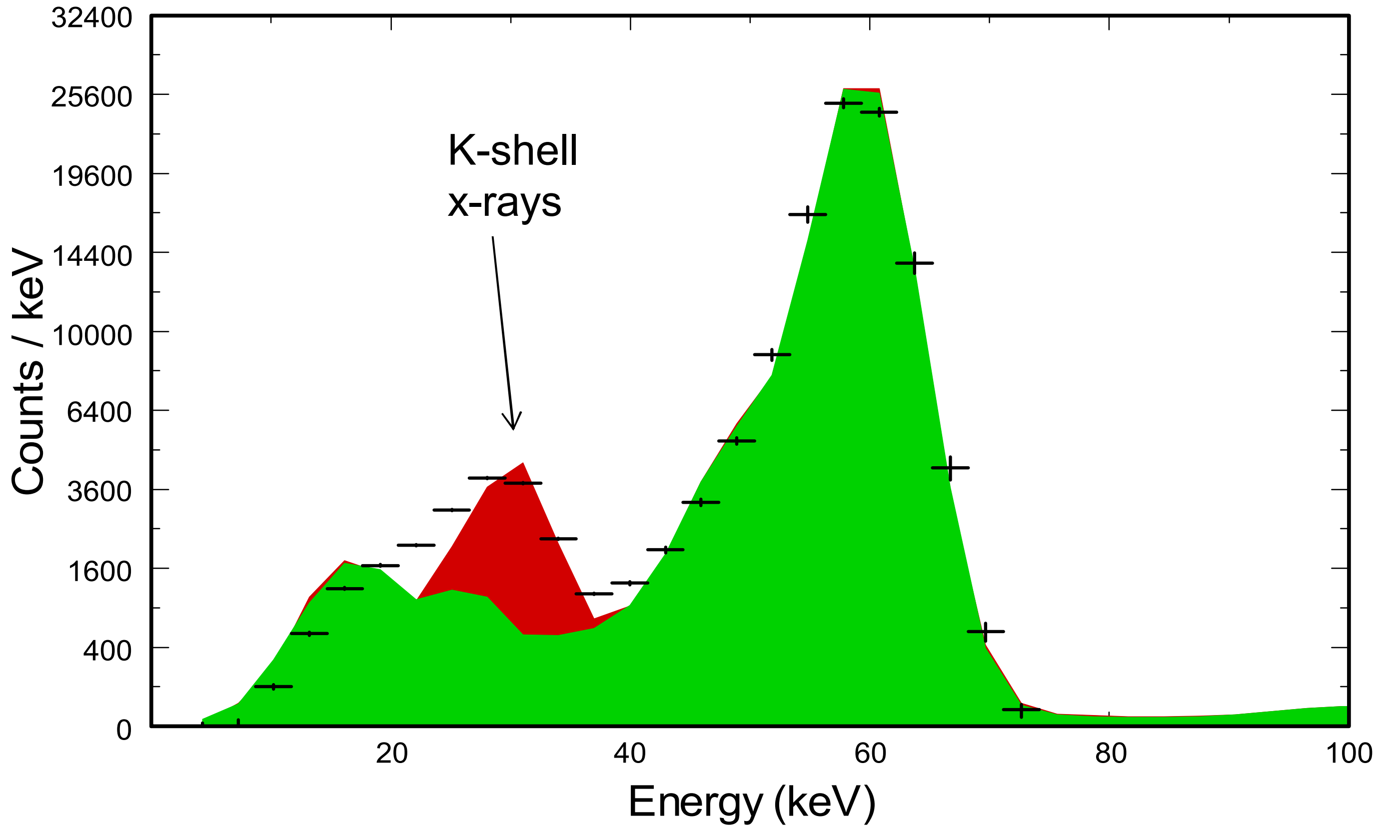
X-Ray Escape Peaks in an NaI Spectrum



- Spectrum for ^{241}Am recorded with an IdentiFINDER-NGH, which contains a 1.4″×2″ NaI crystal
  - The x-ray escape peak could easily be mistaken as scattering

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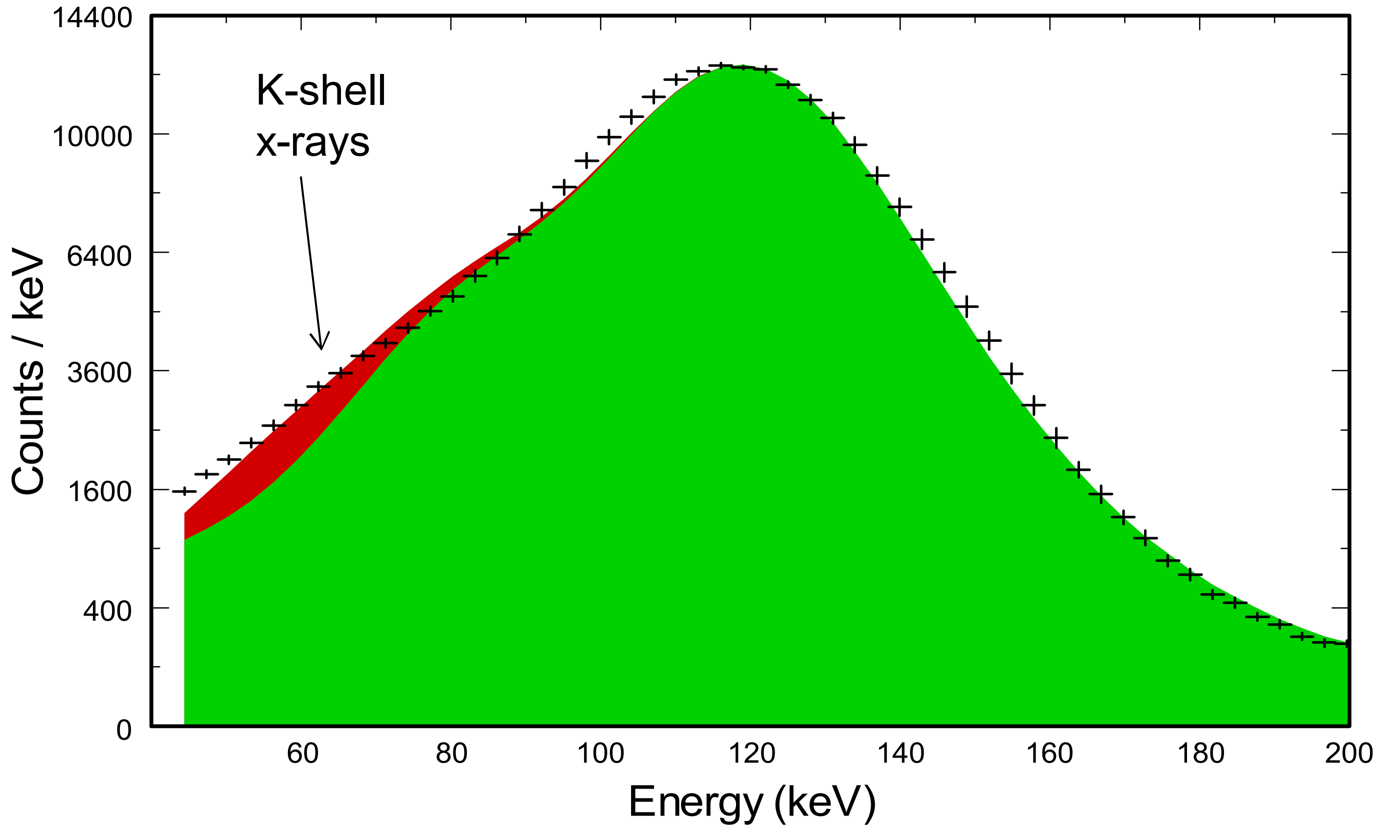
X-Ray Escape Peaks for $CdWO_4$



- Spectrum for ^{57}Co recorded with a 2.3 cm × 2.3 cm × 7.6 cm $CdWO_4$ detector
- The x-ray escape probability moves to higher energies as the K-shell binding energy increases. However, high-Z detectors generally have poor resolution, so x-ray escape features are seldom recognized as x-ray escape peaks

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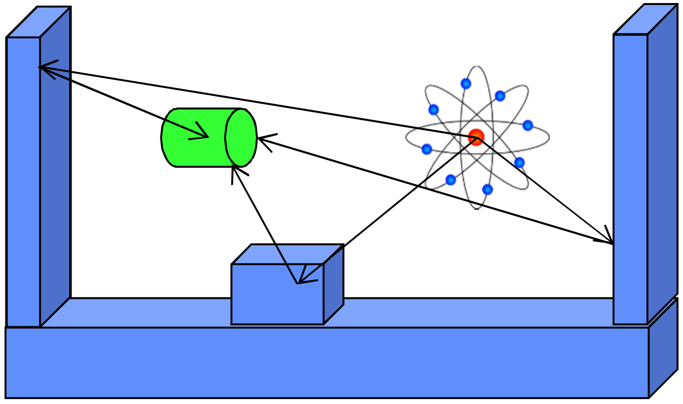
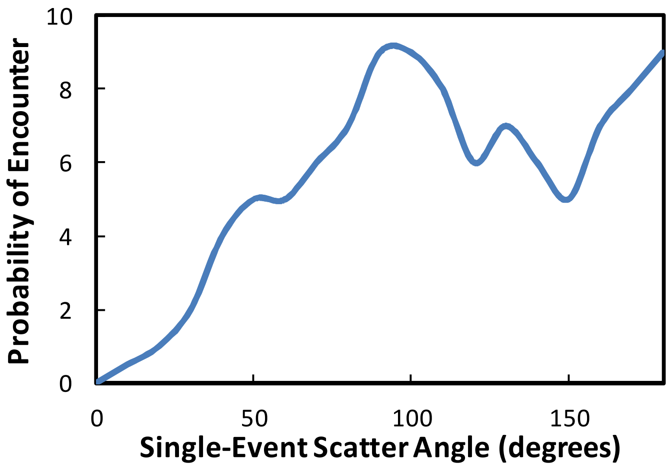
Radiation that Scatters into the Detector

- Scattered radiation is a 3-D problem represented by a 1-D probability vector
- Regardless of whether a photon strikes the wall or the ceiling, the scatter angle dictates the energy of the scattered photon
- The probability is represented as a function of the single-event scatter angle θ
- Average atomic number applied
- A scatter matrix is interpolated to estimate the flux of scattered radiation as a function of $E\gamma$, $E\gamma'$, and θ
- The probability of encountering multiple surfaces is described by a “Clutter” parameter
- Most important systematic parameters are distance and height

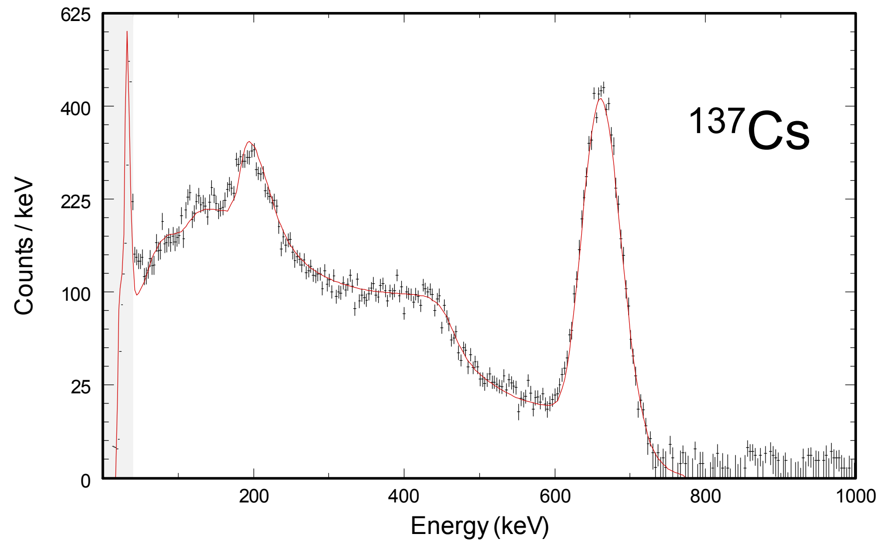


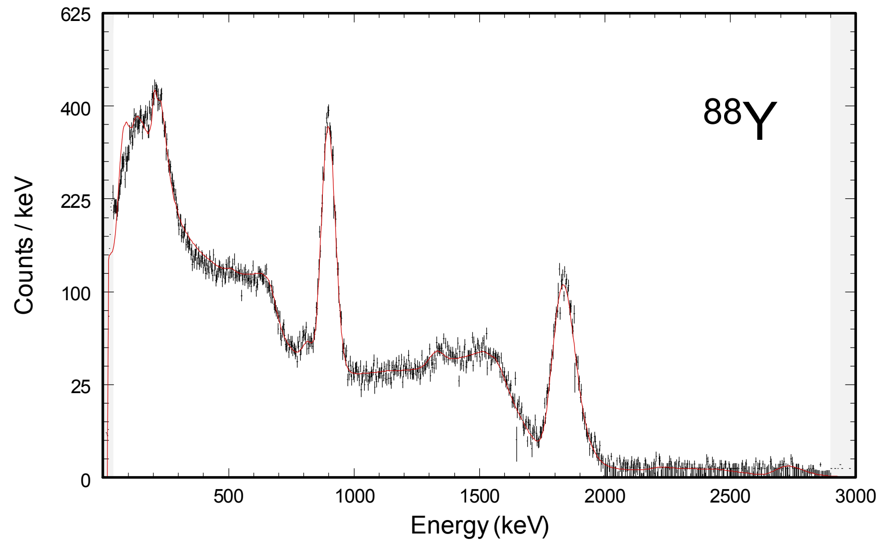


Detector Characterization

Gamma Detector Characterization

- **Define the detector material and dimensions:**
  - Default values for scatter parameters are reasonable estimates in most cases
- **Calibration sources required for accurate characterization of:**
  - Energy calibration
  - Resolution
  - Scatter parameters
- **Typical calibration sources:**
  - ^{133}Ba, ^{137}Cs, ^{60}Co, ^{88}Y, and ^{232}U
- **A nonlinear regression solver is used to determine values of selected parameters**





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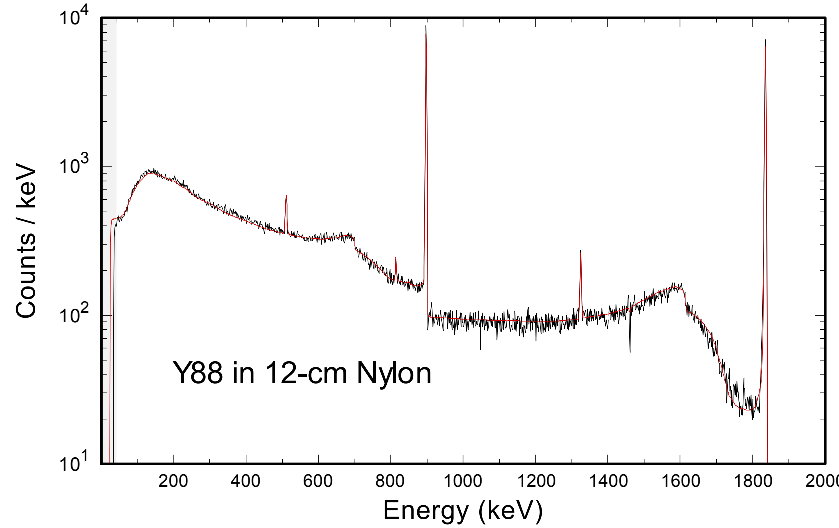
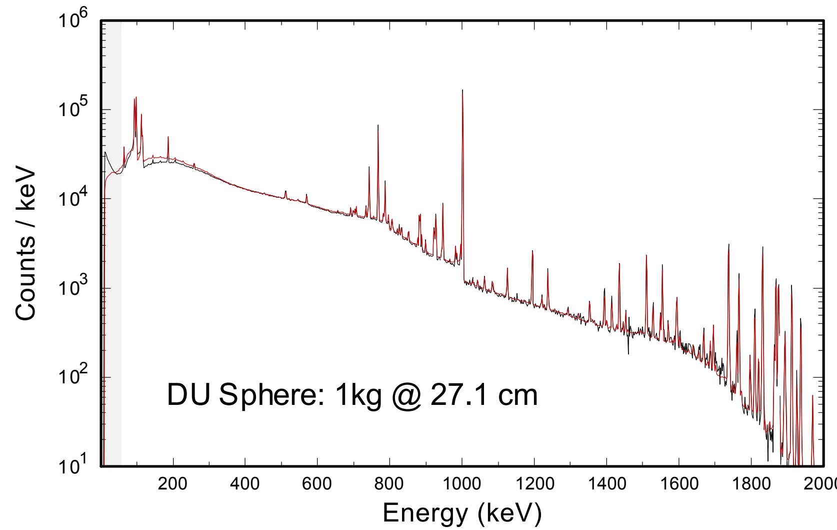
Radiation Transport Integrated with Detector Response

Radiation Transport Approach

- **Discrete Ordinates (DO) calculations use PARTISN and SOURCES4C (LANL)**
  - Gamma and neutron flux in broad groups
  - Volumetric source term as function of location in model
- **RayTrace calculations give leakage of discrete gammas**
  - Retain AN and AD for each gamma
- **RayTrace and DO combined by response function to give best of both**
- **Analytic DRF can be applied to flux computed with codes such as MCNP**
  - Mohini Rawool-Sullivan, “Simulating Authentic Gamma-Ray Spectra: A combined MCNP-GADRAS…”, LA-CP-11-00765 (2011)





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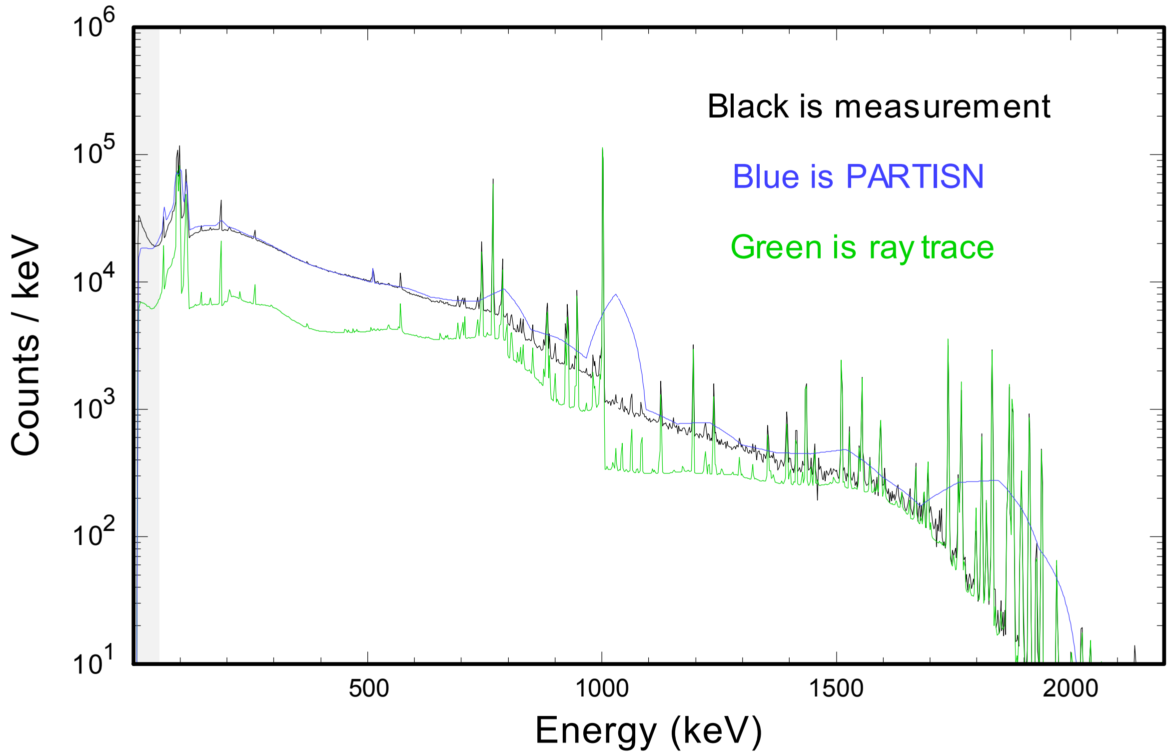
Merging Ray Trace and Discrete Ordinates

This plot compares discrete ordinates (DO) calculation and ray trace calculations with measured spectrum for 1 kg DU sphere.



- **The first step is to strip the uncollided photons from the DO groups**
- **The estimated scatter flux derived from the {AN, AD} for each gamma-ray is stripped from the DO groups**

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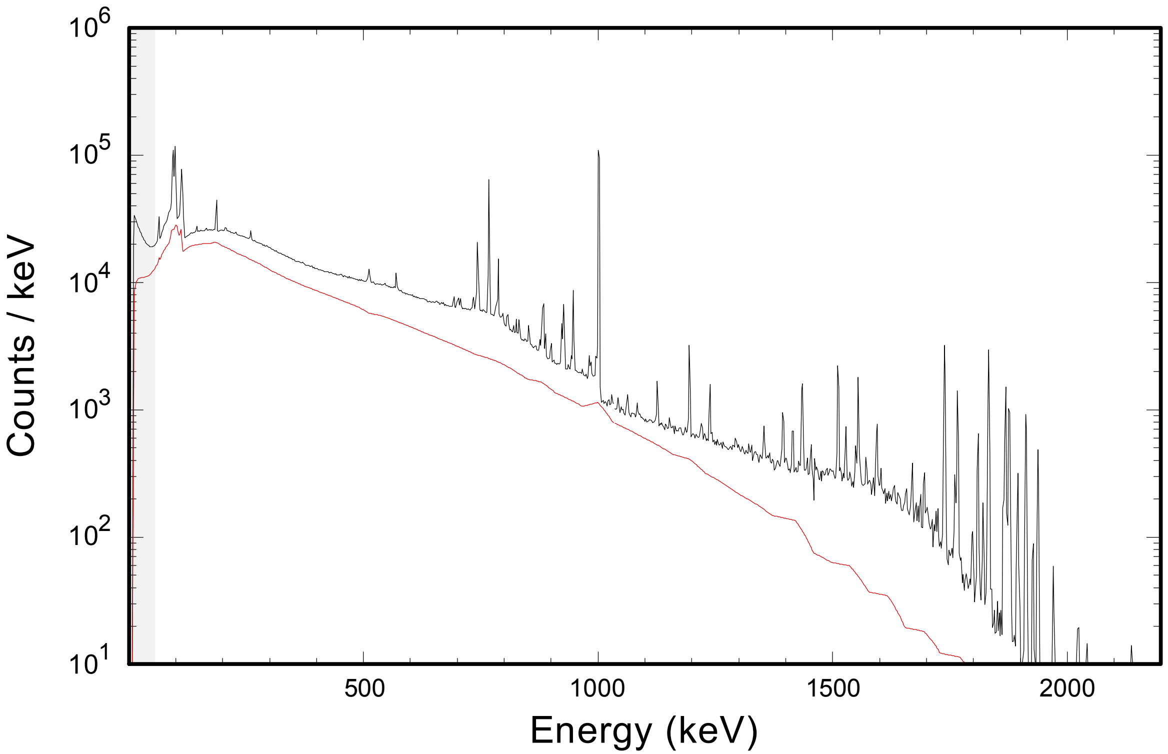
Merging Ray Trace and Discrete Ordinates (continued)

The spectrum that would be derived by applying the DRF to the resulting flux distribution is represented by the red curve to the right



- **Continuum do not contain any discrete features, and can be smoothed**

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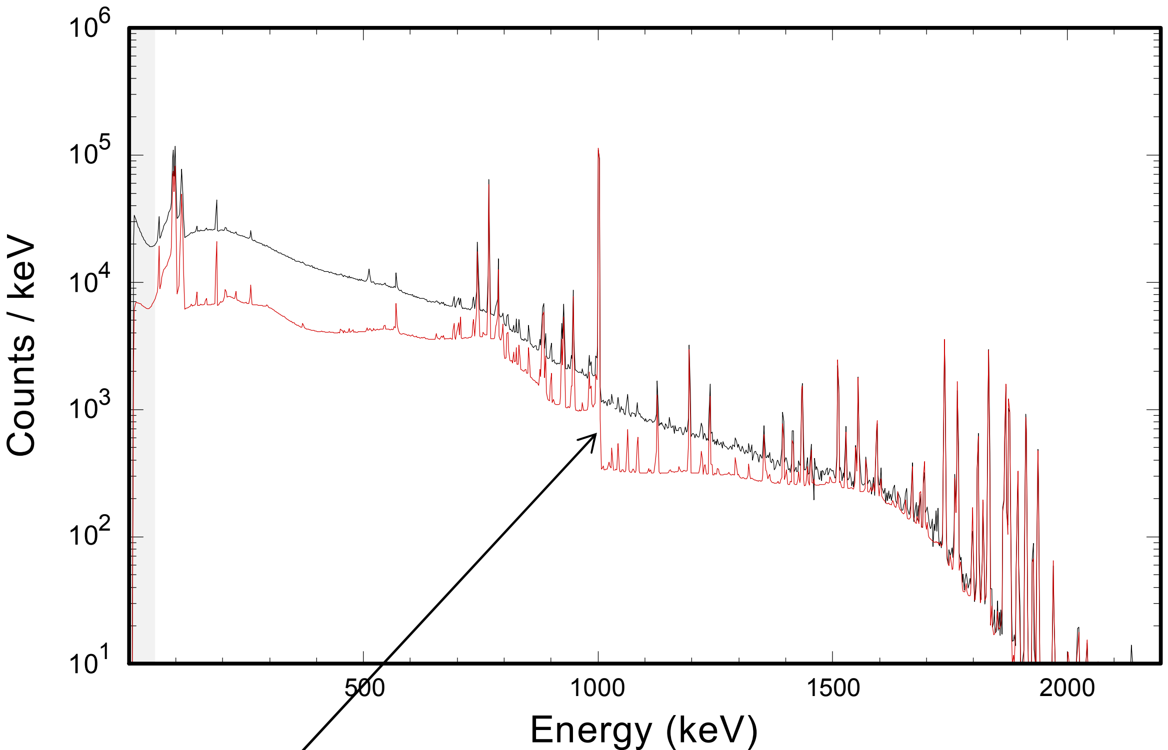

- **Continuum do not contain any discrete features, and can be smoothed**
- **Discrete gammas are processed to derive photopeaks and scatter flux without energy uncertainty**
  - Abrupt changes are associated with low-angle scattering

Merging Ray Trace and Discrete Ordinates (continued)

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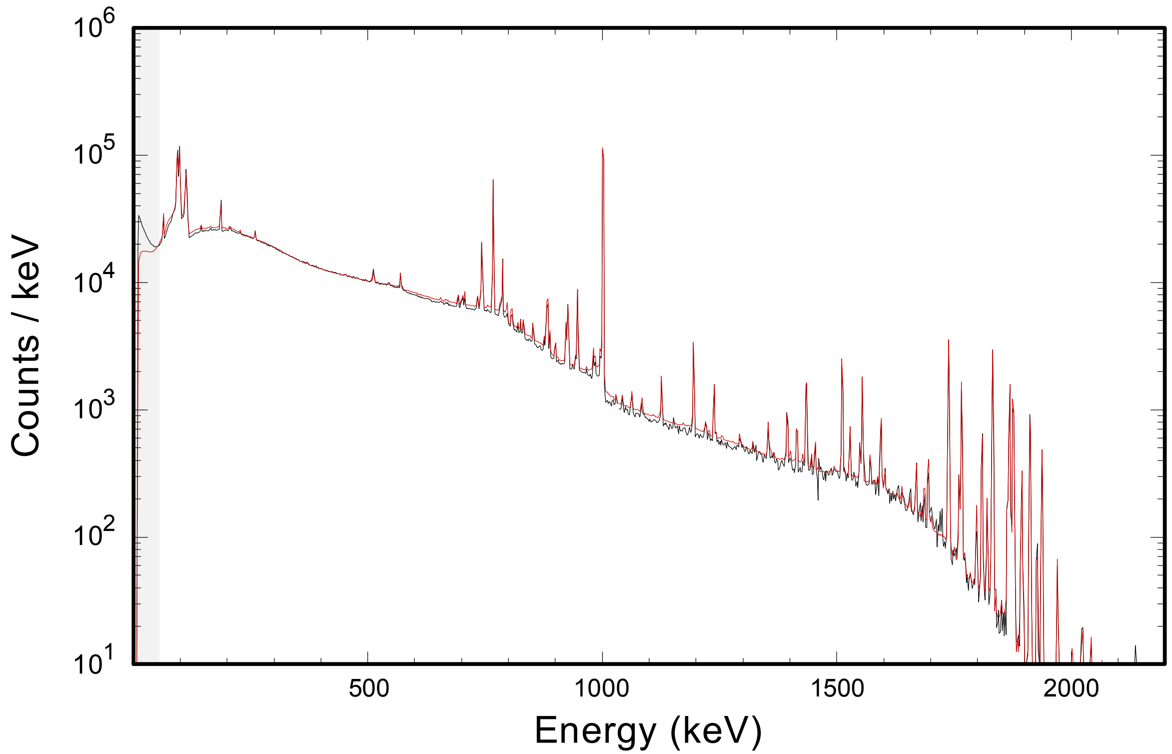

- **Continua do not contain any discrete features, and can be smoothed**
- **Discrete gammas are processed to derive photopeaks and scatter flux without energy uncertainty**
  - Abrupt changes are associated with low-angle scattering
- **The computed spectrum is the sum of the two components**

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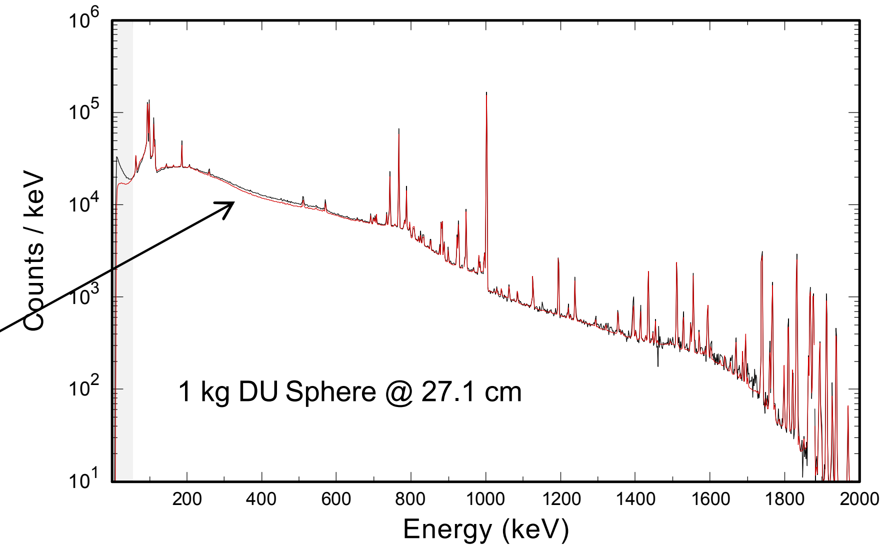
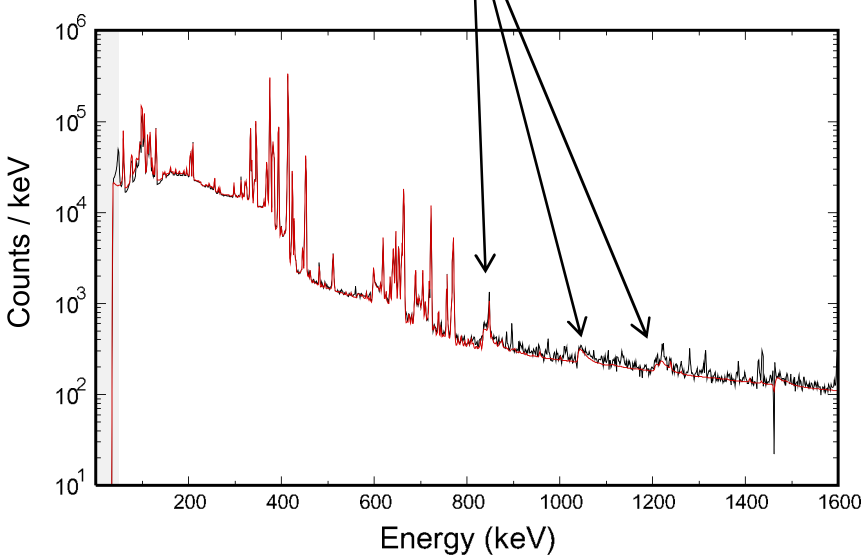
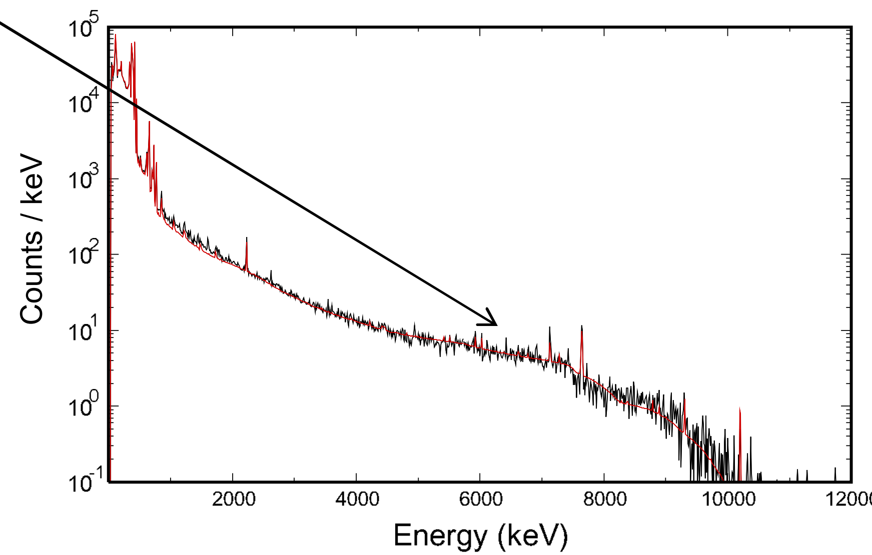
Computational Accuracy

Computational Accuracy Evaluation

- **Computed spectra are accurate for numerous benchmark measurements of calibration sources and spheres**
  - Photopeaks represented well
  - Scatter continuum reproduced
  - Continuum from Bremsstrahlung radiation
  - Neutron inelastic scatter and capture



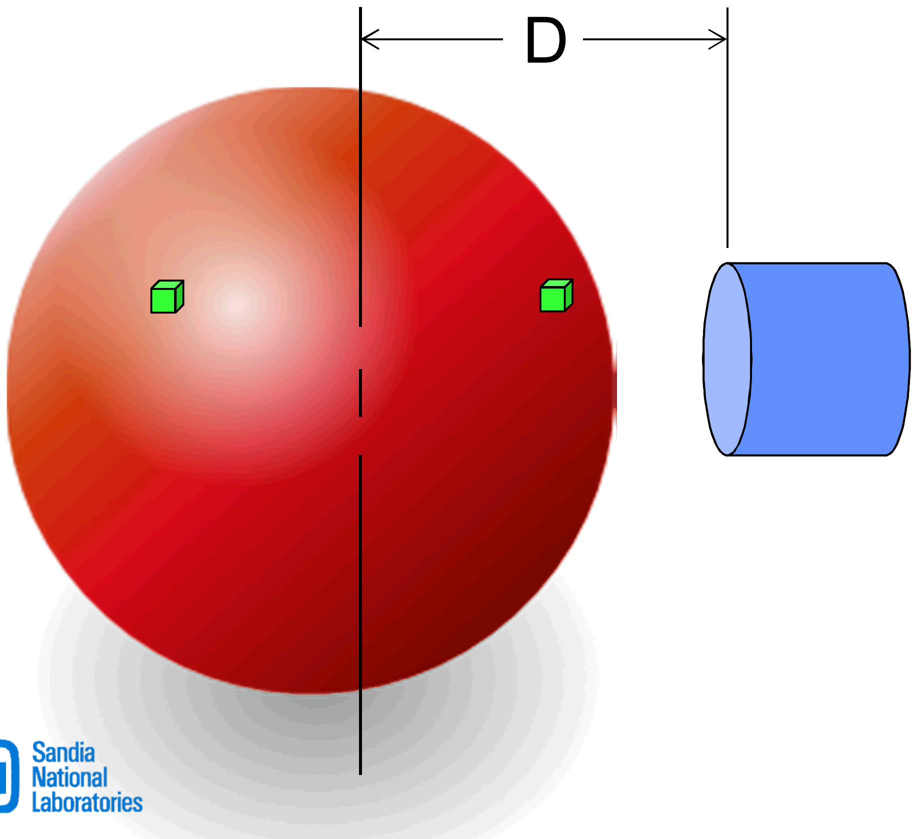


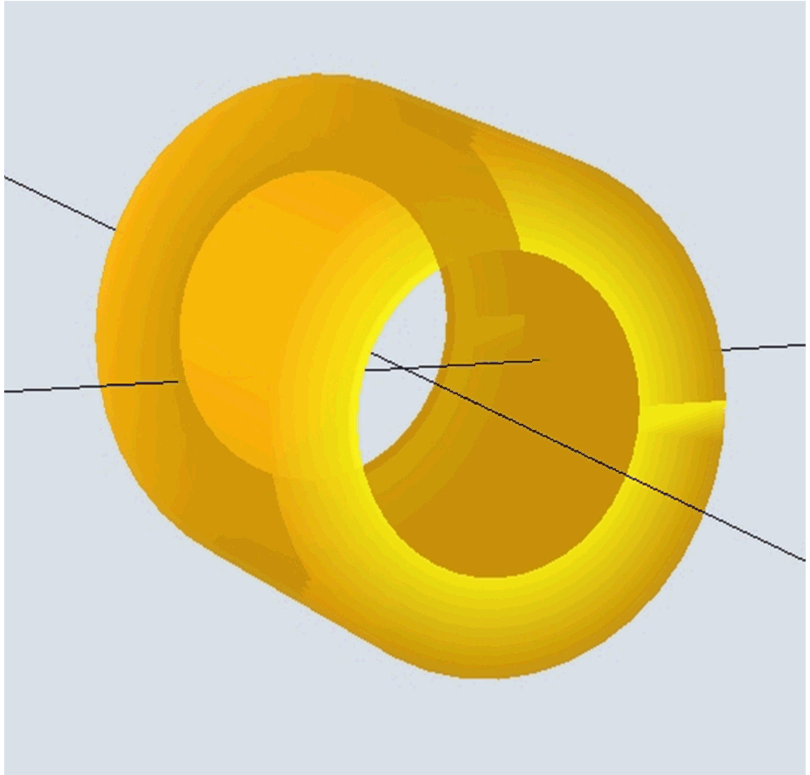


GADRAS: RayTrace3D

GADRAS: RayTrace3D Approach

- **Problem**
  - **Even for spheres, 3-D effects significant when close to the source**
    - The solid angle varies with the location within the source object
    - Radiation may also strike the top and/or sides of the detector
  - **Many objects cannot be represented as spheres**

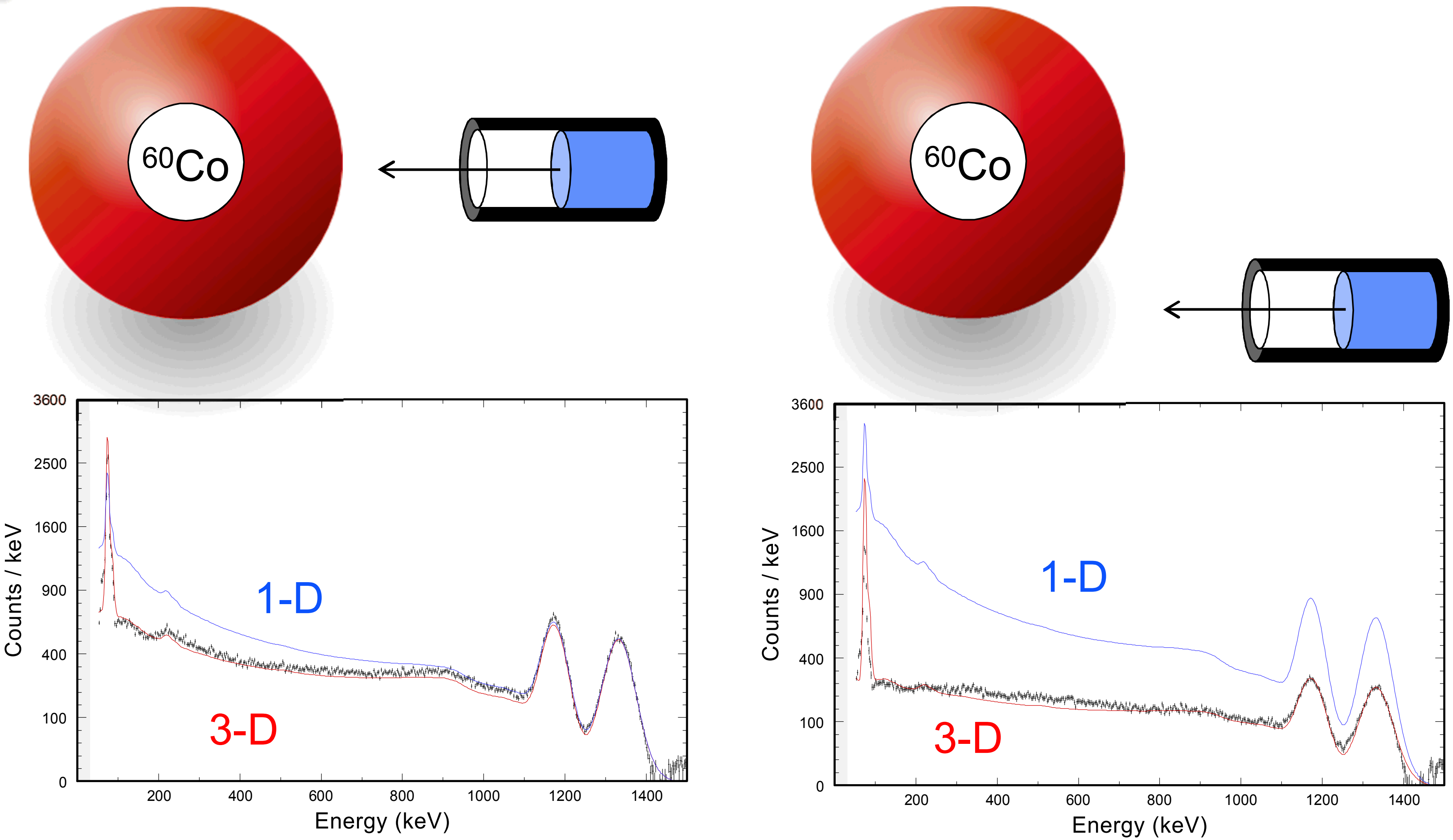




GADRAS: RayTrace3D Approach

- **Solution**
  - Save volumetric source terms so calculation do not need to be repeated for different detectors or when the detector is moved relative to source
    - The emission rates are known everywhere within the model
    - PARTISN gives neutron flux, from which neutron capture gamma ray terms are derived
  - Perform 3-D calculations for un-collided gamma rays by RayTrace3D
  - Estimate the scattered radiation by using {AN, AD} from RayTrace3D
  - Process radiation continuum from Bremsstrahlung in the same way as uncollided gamma rays are treated
    - Volumetric source terms represent both discrete gamma rays and continuum source
- **While we're at it, enable the following**
  - Calculations for collimated detectors
  - Displacement relative to normal in both horizontal and vertical directions
  - Spherical sources embedded in slab or cylindrical configurations
    - Intrinsic radiation and Bremsstrahlung source terms do not change with geometry, so radiation from slabs and cylinders can be computed based on spherical source terms
- **Do it all in under 1 minute**

Collimated Detector

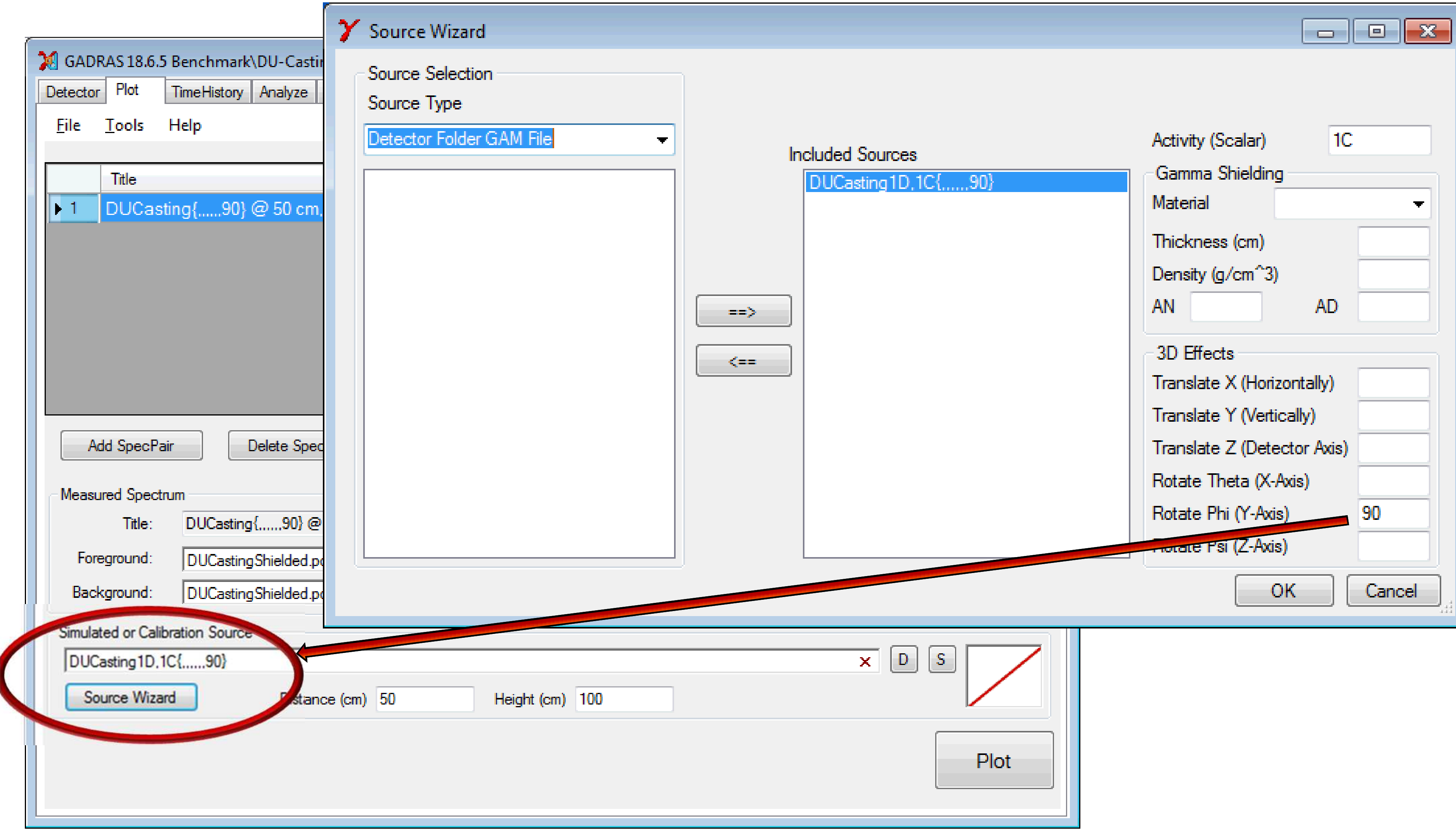


Offset=0

Offset=18 cm

Shorthand Notation and Source Wizard

$\{AN, AD, \delta x, \delta y, \delta z, \theta, \varphi, \psi\}$



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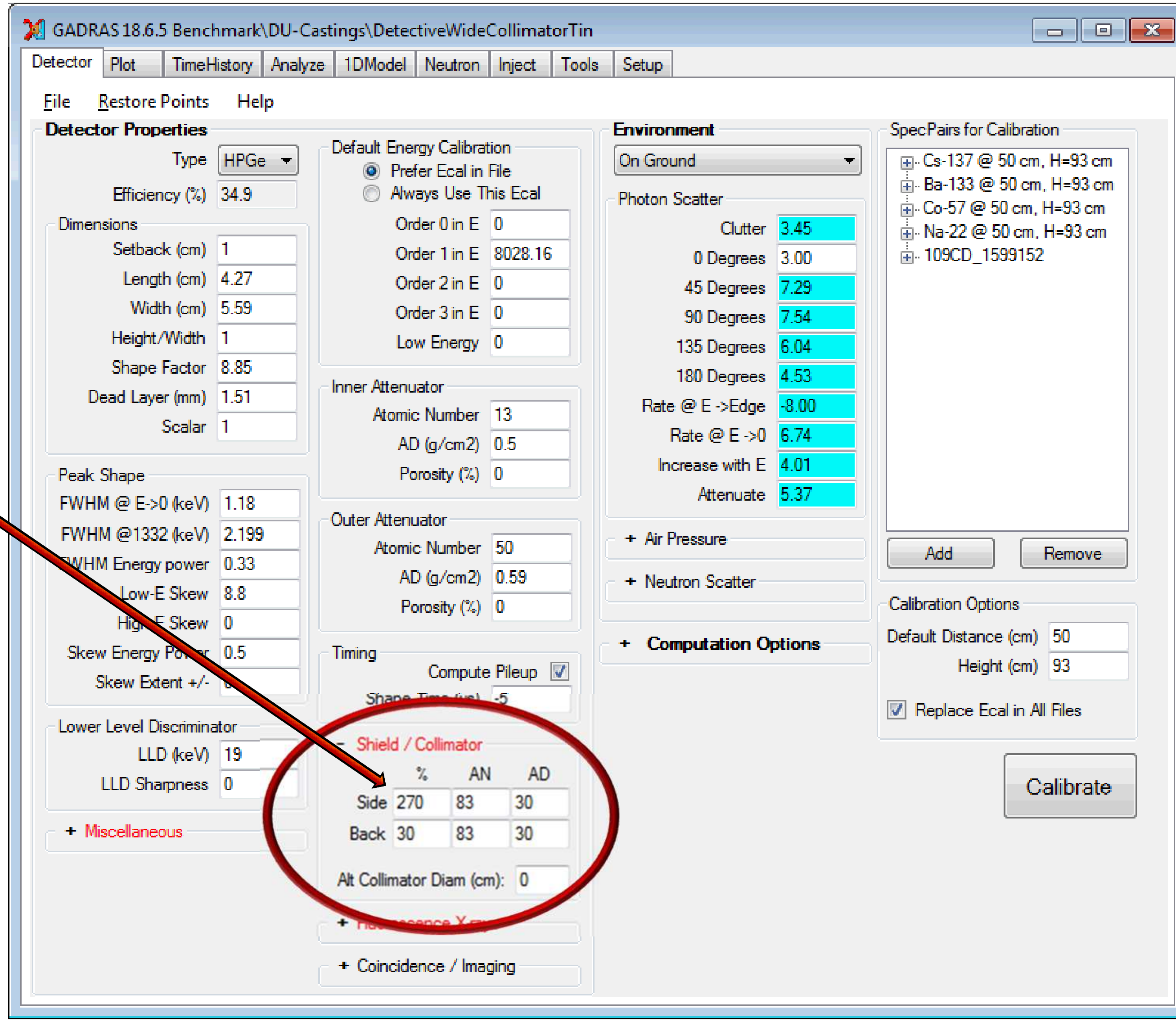
Collimators Defined as Extensions of Side Shields

- 100% defines shield that covers the sides of a detector
- 270%, as in this example, specifies shield extending in front of the detector by 1.7 × detector length
- The atomic numbers and areal densities of shielding materials are specified here
- Shielding affects scatter and has big impact on computed backgrounds



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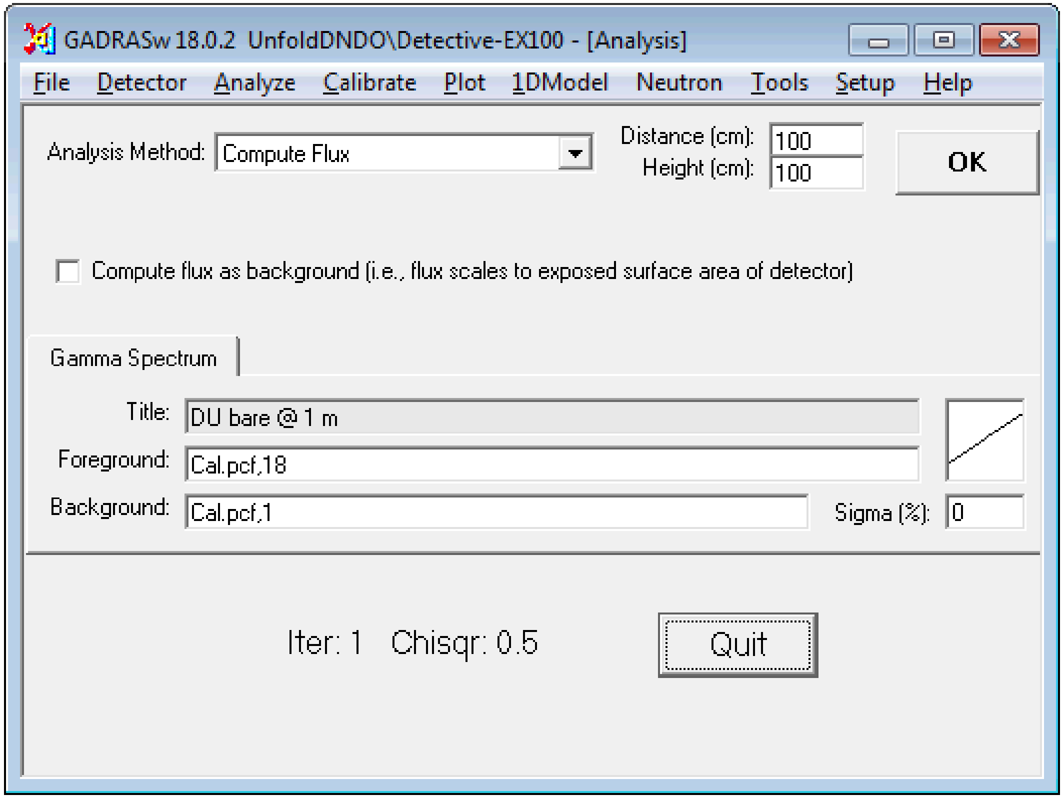
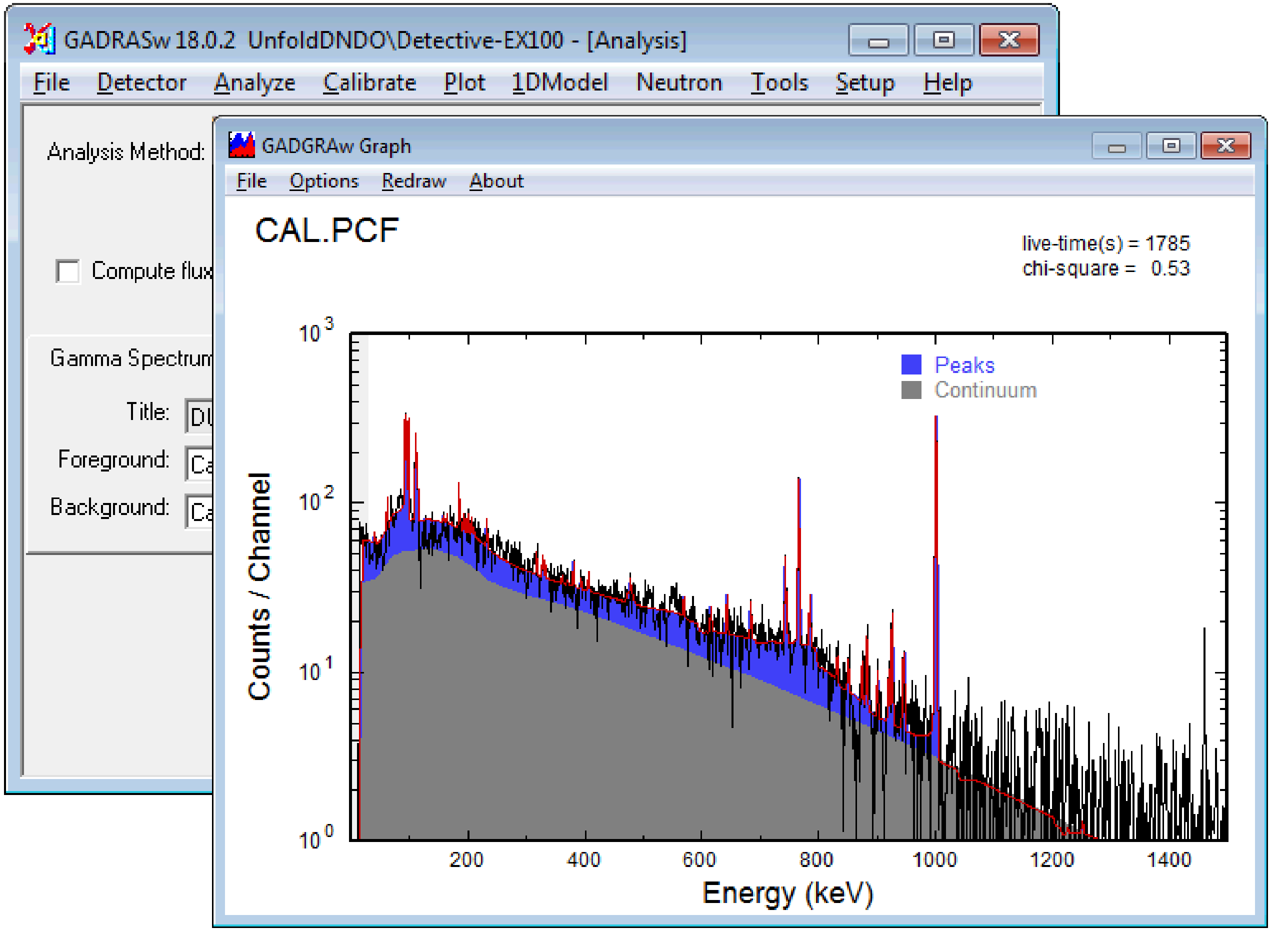
Spectrum Unfolding

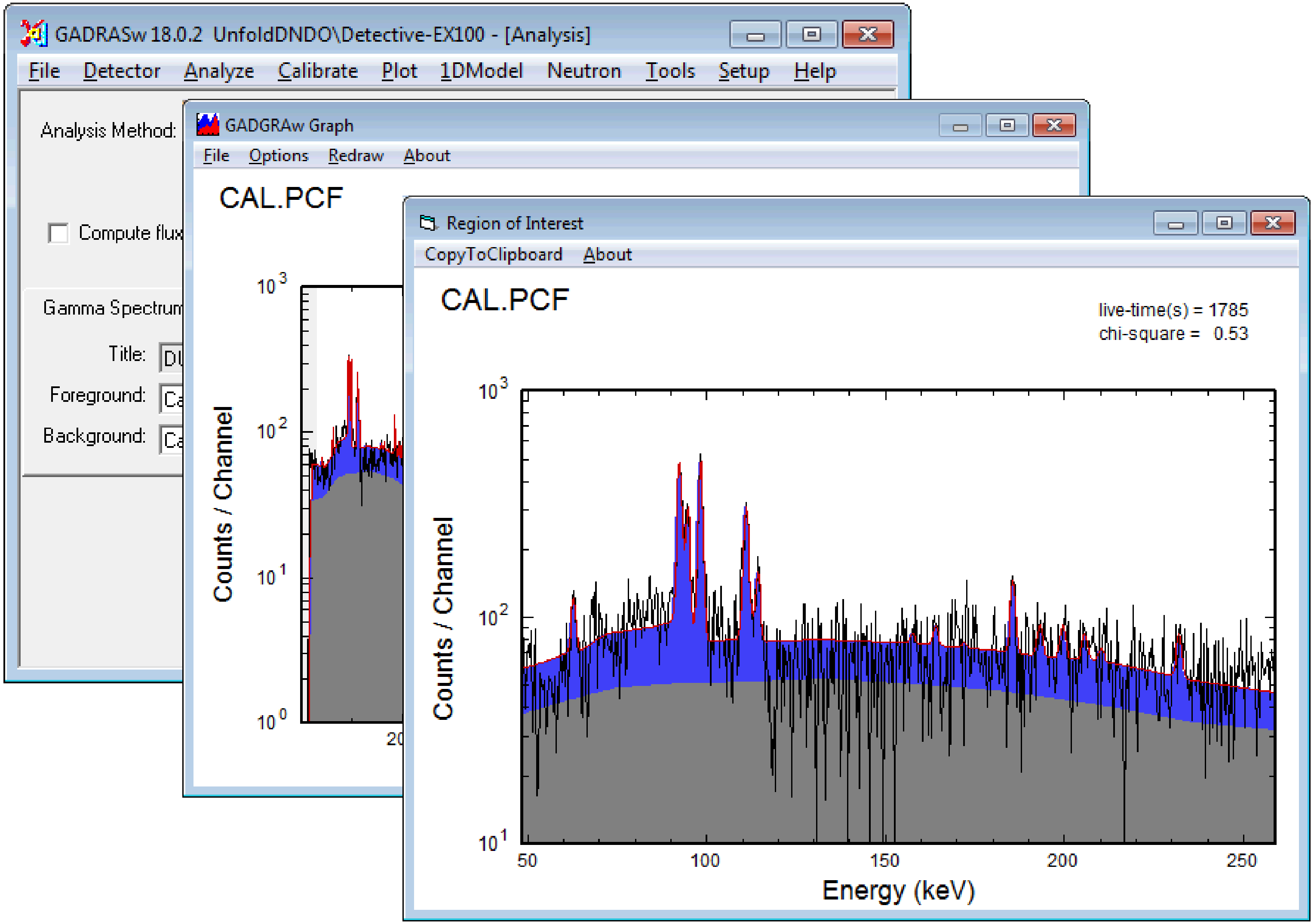
Compute Flux Analysis Method



Compute Flux Analysis Method



Compute Flux Analysis Method



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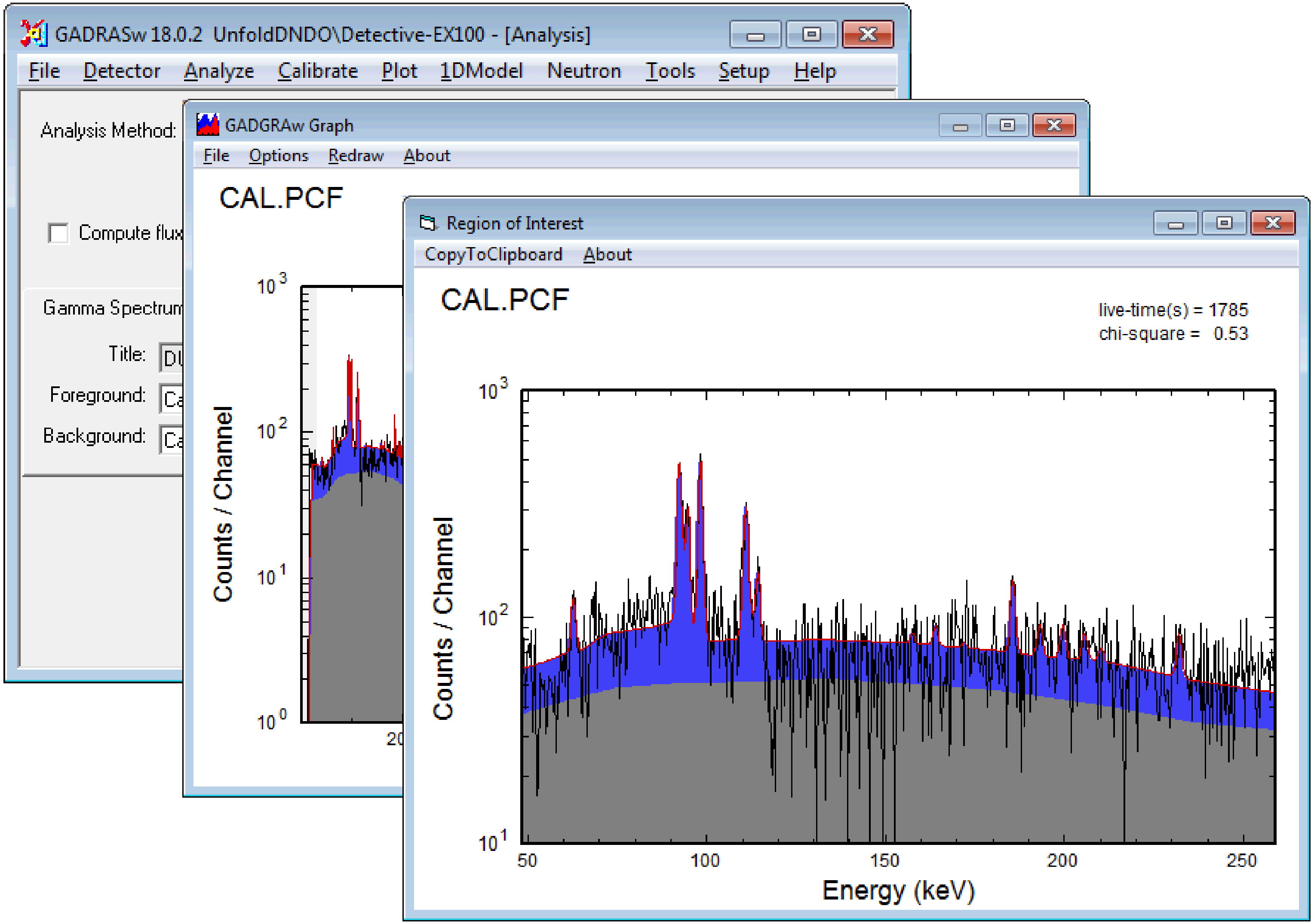
Compute Flux Analysis Method



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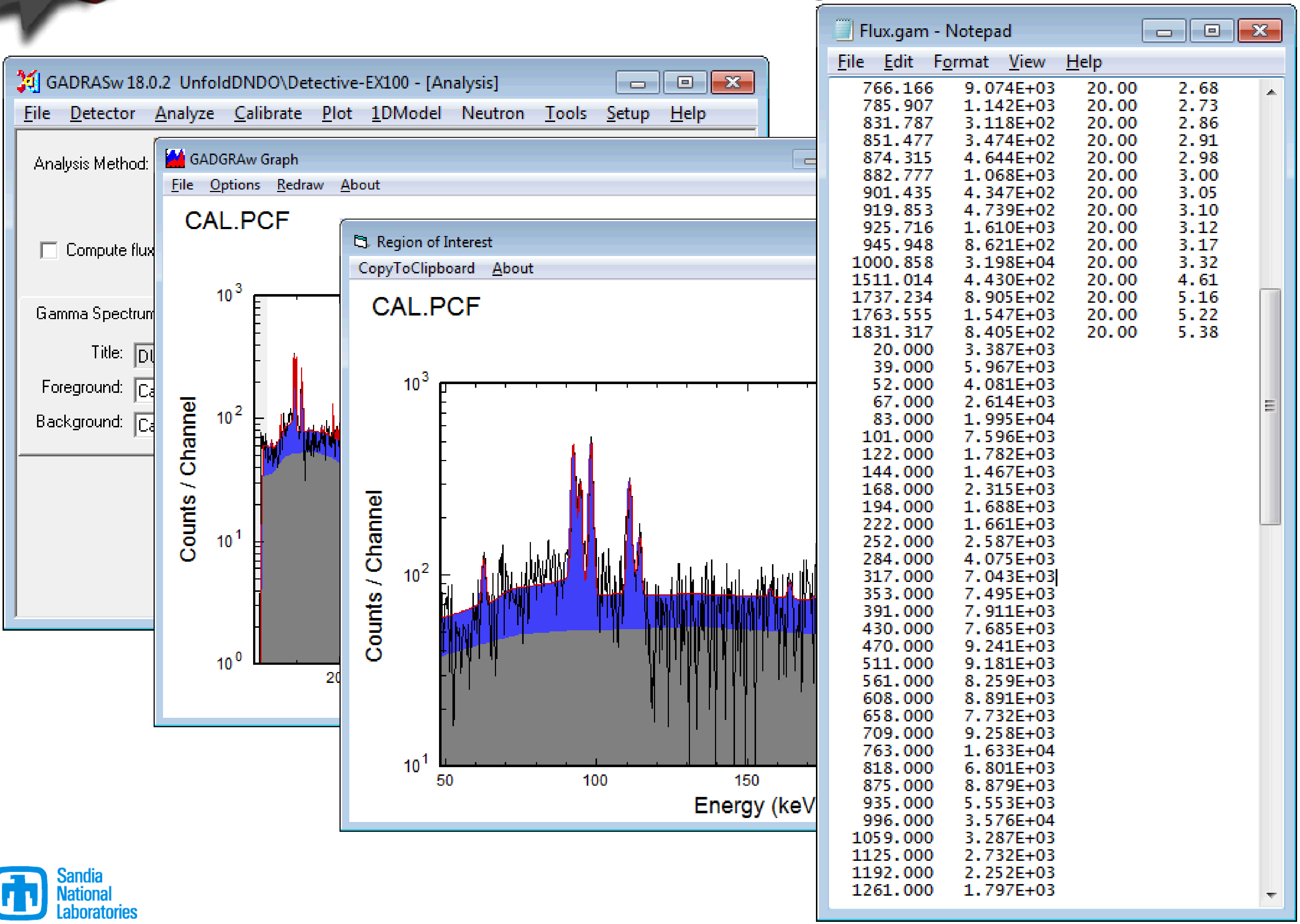
Compute Flux Analysis Method



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Compute Flux Analysis Method

Uncollided Gamma Rays:
Energy Leakage AN AD

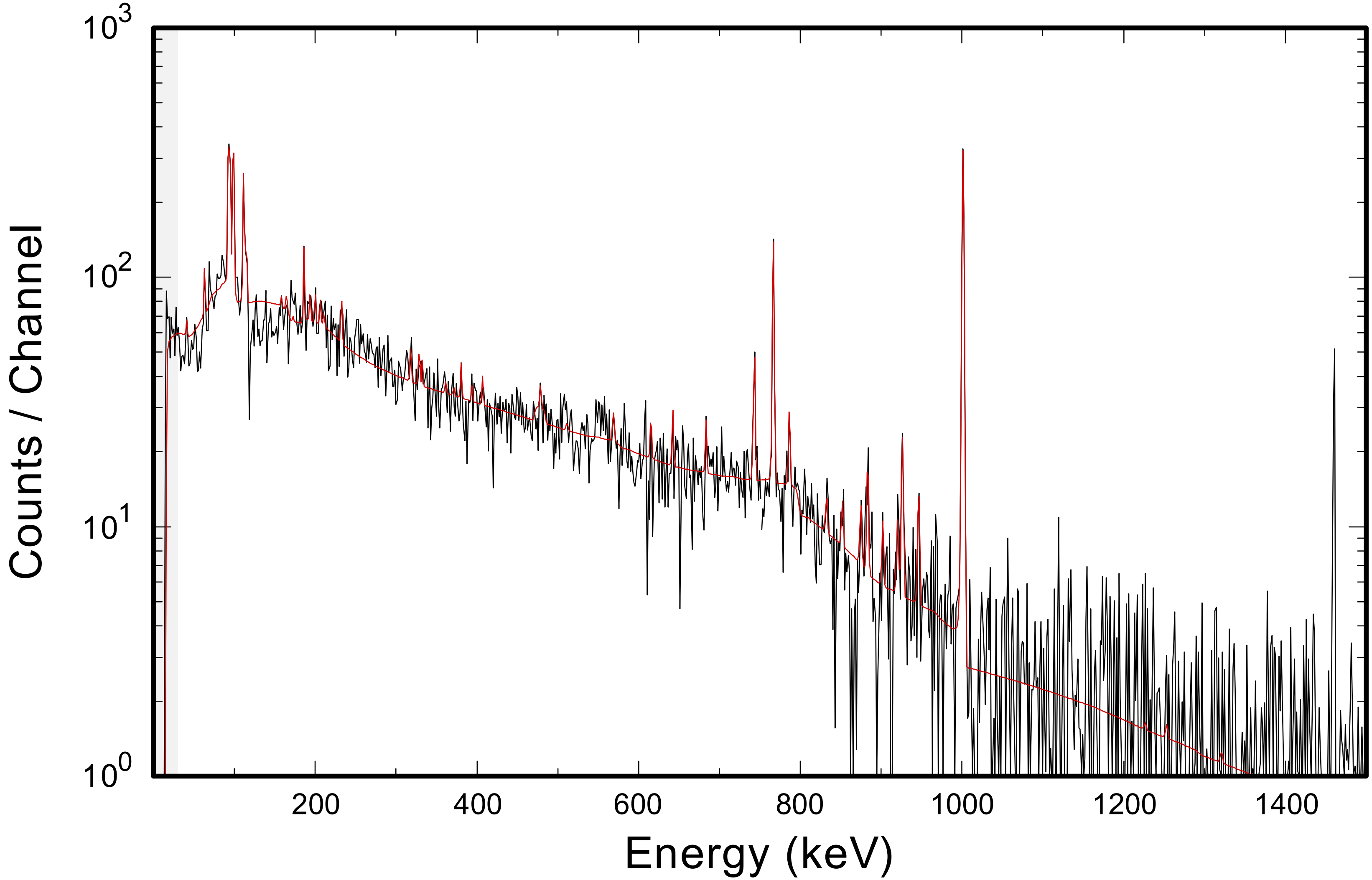
Continuum Groups:
Energy Boundaries Leakage

Flux.gam - Notepad

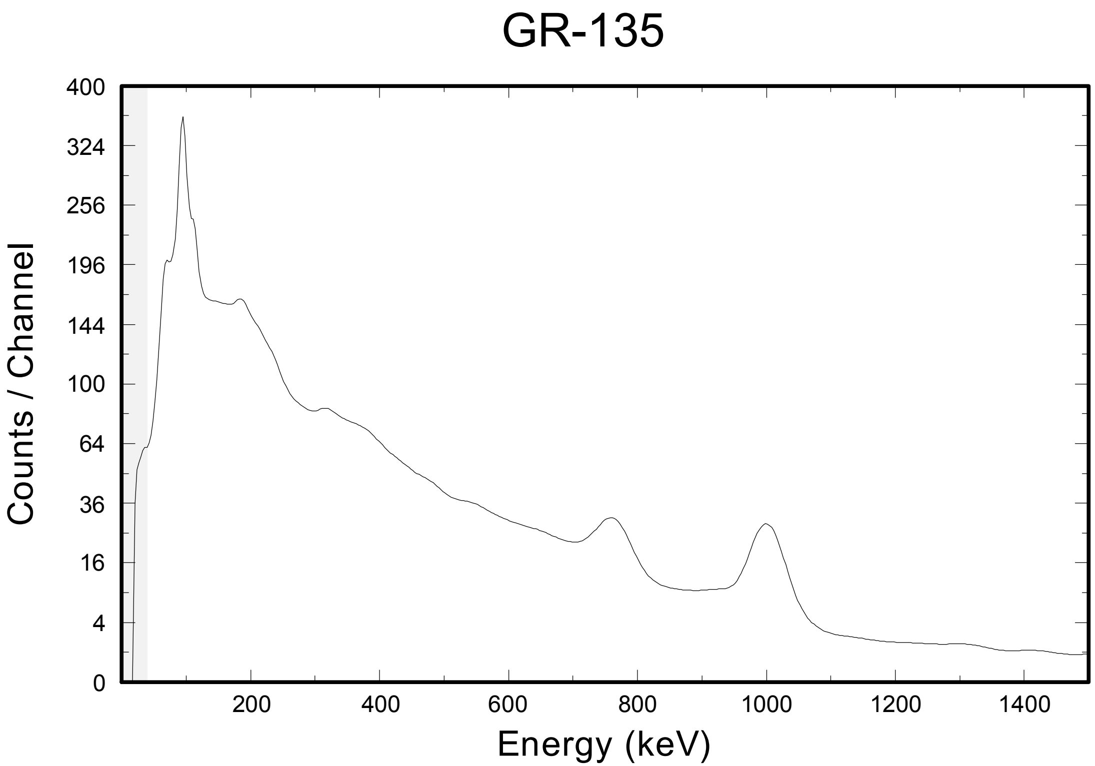
File Edit Format View Help

766.166	9.074E+03	20.00	2.68
785.907	1.142E+03	20.00	2.73
831.787	3.118E+02	20.00	2.86
851.477	3.474E+02	20.00	2.91
874.315	4.644E+02	20.00	2.98
882.777	1.068E+03	20.00	3.00
901.435	4.347E+02	20.00	3.05
919.853	4.739E+02	20.00	3.10
925.716	1.610E+03	20.00	3.12
945.948	8.621E+02	20.00	3.17
1000.858	3.198E+04	20.00	3.32
1511.014	4.430E+02	20.00	4.61
1737.234	8.905E+02	20.00	5.16
1763.555	1.547E+03	20.00	5.22
1831.317	8.405E+02	20.00	5.38
20.000	3.387E+03		
39.000	5.967E+03		
52.000	4.081E+03		
67.000	2.614E+03		
83.000	1.995E+04		
101.000	7.596E+03		
122.000	1.782E+03		
144.000	1.467E+03		
168.000	2.315E+03		
194.000	1.688E+03		
222.000	1.661E+03		
252.000	2.587E+03		
284.000	4.075E+03		
317.000	7.043E+03		
353.000	7.495E+03		
391.000	7.911E+03		
430.000	7.685E+03		
470.000	9.241E+03		
511.000	9.181E+03		
561.000	8.259E+03		
608.000	8.891E+03		
658.000	7.732E+03		
709.000	9.258E+03		
763.000	1.633E+04		
818.000	6.801E+03		
875.000	8.879E+03		
935.000	5.553E+03		
996.000	3.576E+04		
1059.000	3.287E+03		
1125.000	2.732E+03		
1192.000	2.252E+03		
1261.000	1.797E+03		

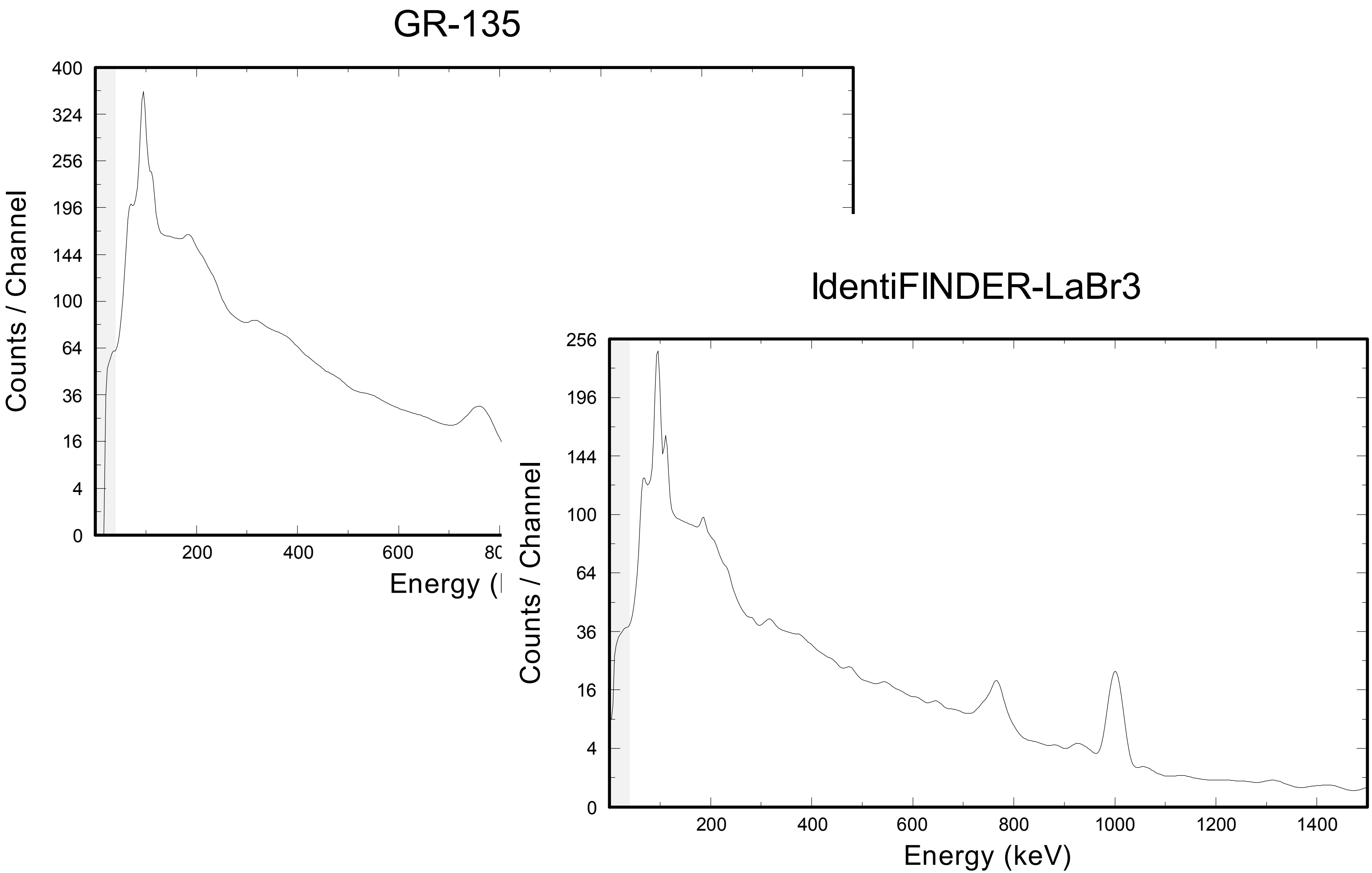
Flux File Processed to Compute Spectrum



Synthetic Spectrum for Another Detector



Synthetic Spectrum for Another Detector



Summary

- **Detector response functions (DRF) enable fast and accurate calculations of gamma-ray spectra**
- **Most interactions are modeled analytically; some performed by Monte Carlo and interpolated subsequently**
- **Radiation transport calculations are coupled with the DRF**
  - 1D transport calculations preserve both continuum and discrete gammas
  - Output from MCNP can be processed with the DRF
- **RayTrace3D calculations are performed if:**
  - The detector is close to source
  - The detector is collimated
  - The detector axis is offset relative to radiation source
  - The source is non-spherical
- **RayTrace3D calculations are completed in seconds, and fully compatible with requirements for analysis algorithms**
- **Spectrum unfolding estimates flux, which can be used to simulate response for other detectors under same conditions**