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Radiation Safety. **Amplified.**

Correlation Effects in Gamma Spectroscopy Efficiency Calibrations and their Impact on Activity and Uncertainty Quantification

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Introduction

- Ongoing effort to improve upon & modernize key analysis functions in Canberra's Genie 2000 gamma spectroscopy software
  - Objective: Consistently provide improvements in algorithms that deliver more accurate, more complete, and more traceable analysis results.
  - Utilize of new technologies and computing capabilities
  - Maintain legacy compatibility with existing algorithms
- Presented today: Correlation effects and impacts on uncertainty
  - Prototype results; Currently undergoing physics validation testing

Why Correlation Effects?

- Application: High Precision Gamma Spectrometry Laboratory Measurements
- Enhanced internal uncertainty propagation to address correlations
  - More accurate uncertainty quantification (UQ)
  - Defendable, mathematically rigorous treatment
  - High confidence in reported uncertainty values
- Enhancements focus on two key analysis stages:
  - Efficiency Calibration
  - Nuclide Identification with Interference Correction

Terminology

- **Correlation** means the errors on two random variables are related to one another
- **Covariance** is a quantitative measure of the degree of relatedness

$$\mathrm{cov}(X_1, X_2) = \langle \delta X_1 \cdot \delta X_2 \rangle \equiv \iint \delta X_1 \delta X_2 \,\mathrm{Pr}(X_1, X_2)\, dX_1 dX_2$$

$$\delta X \equiv (X - \langle X \rangle)$$

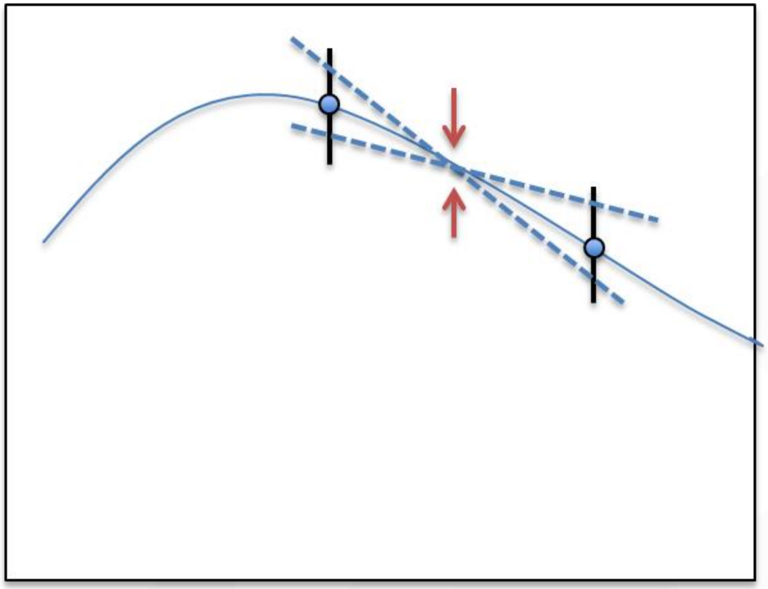
- The **Correlation Coefficient** is a *relative* measure of covariance, between -1 and +1

$$\phi_{1,2} = \frac{\mathrm{cov}(X_1, X_2)}{\sigma(X_1)\sigma(X_2)}$$

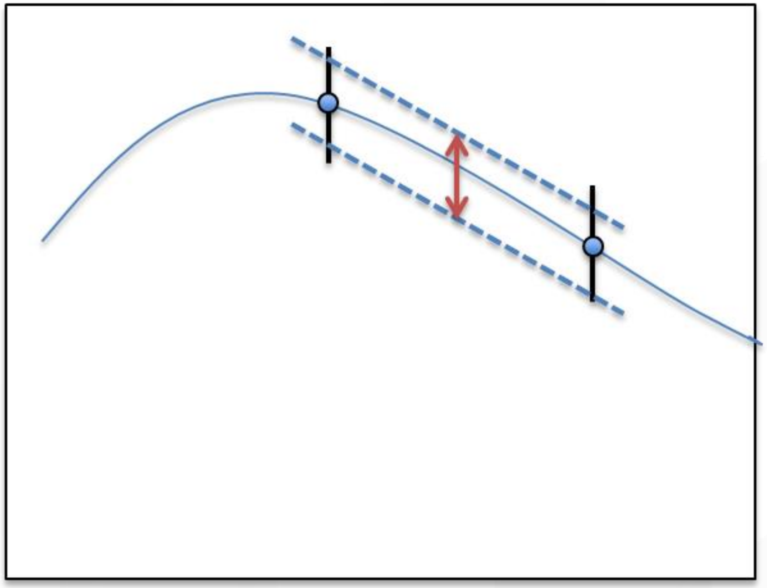
- **Correlations are important when calculating the uncertainty (variance) of a function of random variables:**

$$\sigma^2\big(f(X_1, X_2)\big) = \left(\frac{\partial f}{\partial X_1}\right)^2 \sigma^2(X_1) + \left(\frac{\partial f}{\partial X_2}\right)^2 \sigma^2(X_2) + 2\frac{\partial f}{\partial X_1}\frac{\partial f}{\partial X_2}\mathrm{cov}(X_1, X_2)$$

An intuitive way to think about the effects of covariance



Uncorrelated data vary independently, leading to smaller uncertainties in between data points



Correlated data tend to vary together – both up or both down – leading to larger uncertainties in between data points

Background

- Measurement uncertainty can be underestimated when covariance effects are not accounted for
  - Measured efficiency calibrations with multi-line nuclides
  - Weighted Mean Activities of multi-line sample nuclides
  - Interference correction
- These are all instances of Parameter Estimation (Least Squares Fitting)
  - Combining independent measurements reduces uncertainty
  - Inappropriate when the data are correlated
- Current Options for Genie users:
  - Apply an overestimated measurement Sample Uncertainty
  - “Empirical”, “Interpolated” efficiency models use interpolated uncertainty propagation
  - These may result in a greater than necessary activity uncertainty
- **To directly address correlations, we start to modify the Genie fitting routines used by the algorithms (such as the least squares fitting)**

Least Squares Fitting with Correlations

- To account for correlated input data, Genie algorithm chi-squared calculation is modified
- $1/\sigma^2$ weighting factors are replaced with the inverse covariance matrix of the data V^{-1} :

$$\chi^2 = \sum_{i=1}^{N} \frac{(y_i - \sum a_m f_m(x_i))^2}{\sigma_i^2}$$

becomes

$$\chi^2 = (\vec{\mathbf{y}}(\vec{\mathbf{x}}) - \mathbf{F} \cdot \vec{\mathbf{a}})^{\mathbf{T}} \cdot \mathbf{V}^{-1} \cdot (\vec{\mathbf{y}}(\vec{\mathbf{x}}) - \mathbf{F} \cdot \vec{\mathbf{a}})$$

where

$$\mathbf{V} = \begin{pmatrix} \sigma_1^2 & \mathrm{cov}(y_1, y_2) & \mathrm{cov}(y_1, y_3) \\ \mathrm{cov}(y_2, y_1) & \sigma_2^2 & \mathrm{cov}(y_2, y_3) \\ \mathrm{cov}(y_3, y_1) & \mathrm{cov}(y_3, y_2) & \sigma_3^2 \end{pmatrix}$$

- **Next Step: How to calculate the covariance of the input data**

Correlations in the Measured Efficiency Data

- The Efficiency calibration fits a function to a set of measured "efficiency triplets" $\{E, \varepsilon, \sigma(\varepsilon)\}$

$$\varepsilon_i = \frac{N_i}{I_{ia} A_a T}, \qquad \sigma(\varepsilon_i) = \varepsilon_i \left\{ \frac{\sigma^2(N_i)}{N_i^2} + \frac{\sigma^2(I_{ia})}{I_{ia}^2} + \frac{\sigma^2(A_\alpha)}{A_\alpha^2} \right\}^{1/2}$$

  - Net peak area N_i, gamma ... le Activit A_a, Measureme ... ive Time T
  - Indices i and α specify e ... spec ... y

Calibration Measurement (statistical Unc on this peak)

From the Nuclide Library

From the Source certificate

- Knowing the true correlations is complex and challenging
- Assumption made: Any gamma lines from a common nuclide will be considered 100% Correlated

Correlated Efficiency Calibration Engine

- A modified version of the G2K efficiency calibration algorithm was prototyped in Python
  - **Calculates correlations between measured efficiency data using Measured Efficiency Triplets and Nuclide Library data**
  - Modified Least-Squares fitting routine correctly incorporates data correlation matrix
  - Outputs Efficiency Model Parameters and Parameter Covariance Matrix, which are stored in spectral data file
- No need for user to calculate or enter correlations
- Parameter Covariance Matrix data is available to be used in downstream analysis, if needed
  - Used to calculate uncertainties of calculated efficiency values
  - Used to calculate correlations between calculated efficiencies
  - Parameters are always correlated, even if input data isn't!
- Algorithm tested using simulated data (shown next)

Efficiency Calibration Examples – Testing Approach

- Efficiency Calibrations were created using simulated data, both with and without accounting for effects of data correlations.
- Three calibration standards with differing degrees of correlation,
  - 3% (1σ) Activity Uncertainty on each nuclide

Nuclide	Energy
Am-241	59.5
Cd-109	88.0
Co-57	122.1
Ce-139	165.9
Sn-113	391.7
Cs-137	661.7
Mn-54	834.8
Y-88	898.0 1836.0
Co-60	1173.2 1332.5

"Mixed Gamma"

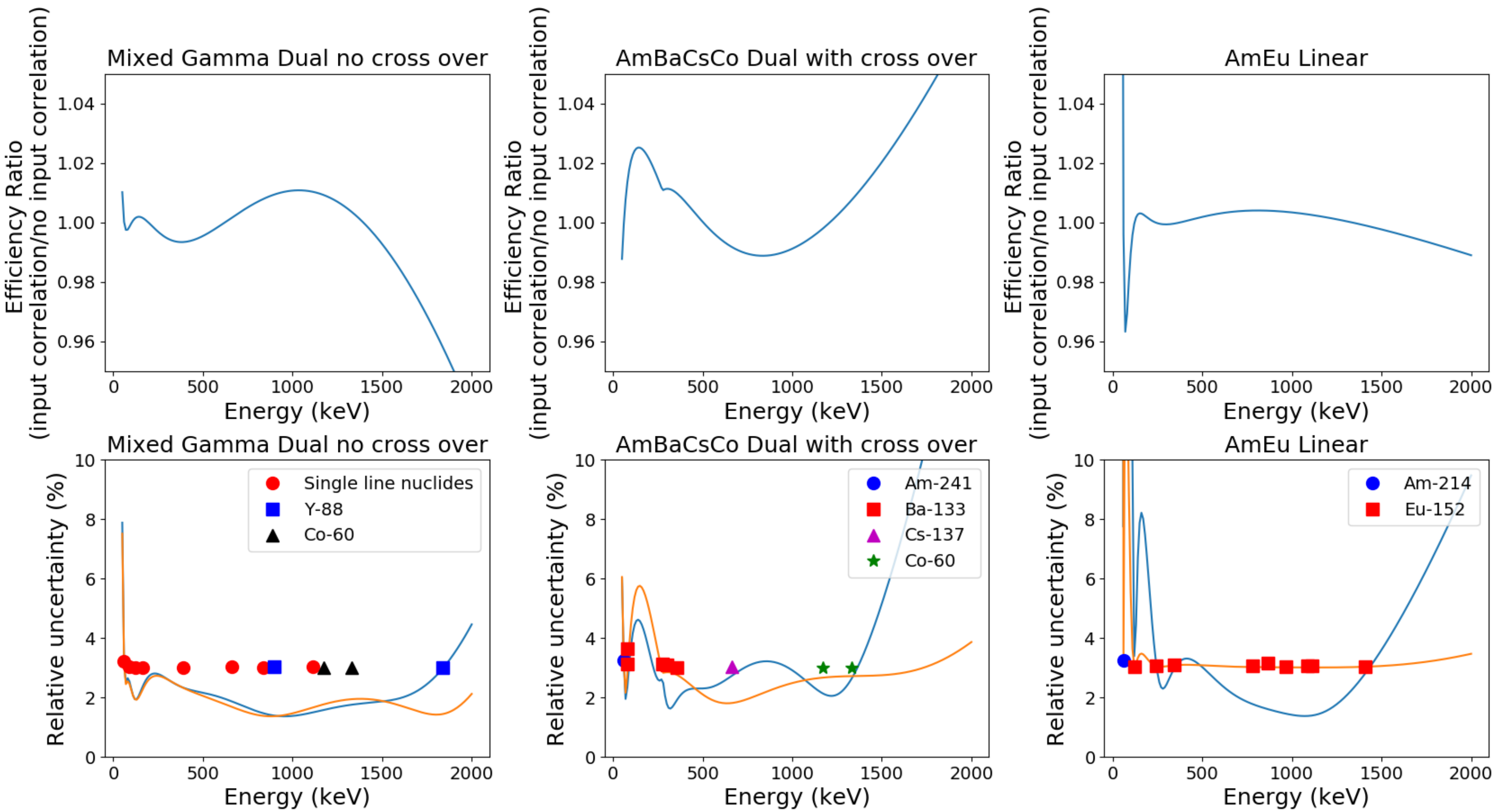
Nuclide	Energy
Am-241	59.6
Ba-133	79.6 81.0 276.4 302.8 356.0 383.9
Cs-137	661.7
Co-60	1173.2 1332.5

"AmBaCsCo"

Nuclide	Energy
Am-241	59.6
Eu-152	121.8 244.7 344.3 778.9 867.3 964.0 1085.8 1112.0 1408.0

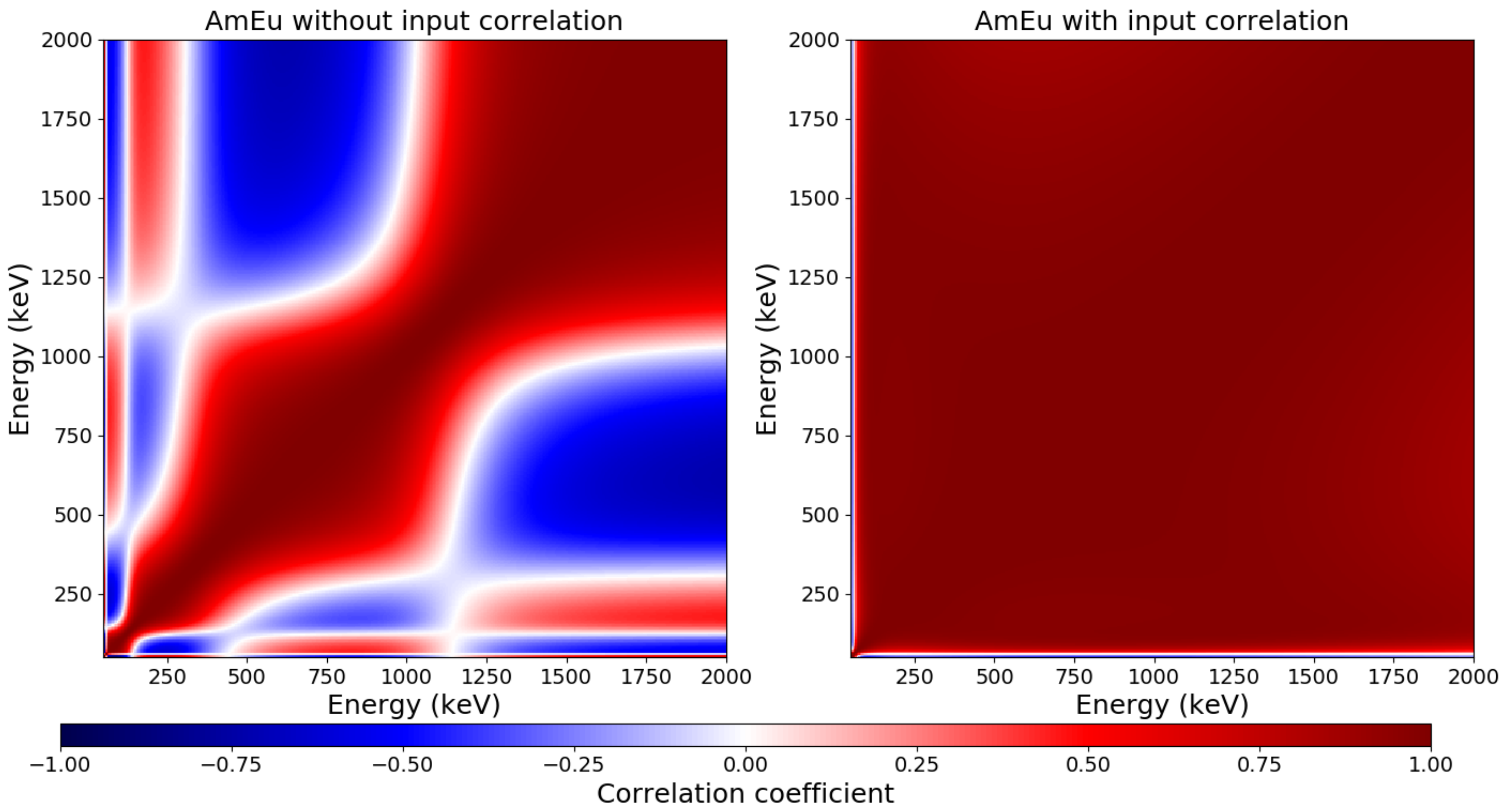
"AmEu"

Changes in Efficiency and Uncertainty with Correlated Data



Ratios of efficiency values calculated with and without source standard correlations (top); Efficiency uncertainties with (orange) and without (blue) source standard correlations

Correlations Between Calculated Efficiencies



The **Correlation Coefficient** is a *relative* measure of covariance, between -1 and +1

$$\phi_{1,2} = \frac{\text{cov}(\varepsilon_1, \varepsilon_2)}{\sigma(\varepsilon_1)\sigma(\varepsilon_2)}$$

NID with Interference Correction Engine

- A New Version of the Genie 2000 NID with Interference Correction Algorithm was also prototyped in Python
  - Calculates correlations between measured nuclide line activities using measured data and correlations between calculated efficiency values

$$V_{ij} = \frac{N_i N_j}{\varepsilon_i \varepsilon_j} \frac{\mathrm{cov}(\varepsilon_i, \varepsilon_j)}{\varepsilon_i \varepsilon_j}$$

  - Modified Least-Squares fitting routine correctly incorporates data correlation matrix for Weighted Mean Activity and Interference Correction fits.

$$\chi^2 = \sum_{ij} \left(\frac{N_i}{\varepsilon_i} - \sum_{\alpha} A_\alpha I_{\alpha i} \right) V_{ij}^{-1} \left(\frac{N_j}{\varepsilon_j} - \sum_{\beta} A_\beta I_{\beta j} \right)$$

  - Outputs: Weighted Mean Activities and Weighted Mean Activity Uncertainties, which are stored in spectral data file
- No need for User to calculate or enter correlations
- Algorithm tested using simulated data (shown next)

Weighted Mean NID Examples: Testing Approach

- Five simulated sample spectra were created for multi-line nuclides to demonstrate the effects of correlations on NID activity uncertainties
- Each Spectra was analyzed with each of the three calibrations:
  - I. Mixed Gamma (Low Corrlation),
  - II. AmBaCsCo (medium Correlation),
  - III. AmEu (High Correlation)
- Counting uncertainties small compared to efficiency uncertainties
- NID Analysis was performed with:
  1. Genie Today (no correlations),
  2. New Fitting method with ability to take into account correlations (but no input efficiency correlations identified),
  3. New fitting method & efficiency input correlations identified.

Sample nuclides and energies for NID spectra

Nuclide	Energy
CO-60	1173.2
	1332.5

Nuclide	Energy
CO-57	122
	137

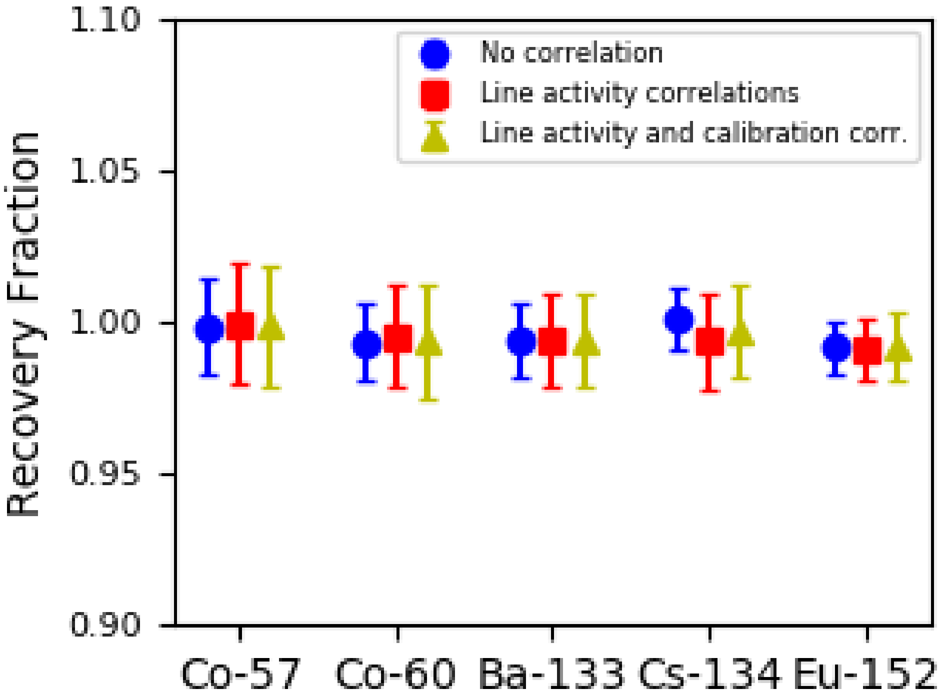
Nuclide	Energy
BA-133	79.6
	81.0
	276.4
	302.8
	356.0
	383.9

Nuclide	Energy
CS-134	475.4
	563.2
	569.3
	604.7
	795.9
	802.0
	1168.0

Nuclide	Energy
Eu-152	121.8
	244.7
	344.3
	778.9
	867.3
	964.0
	1085.8
	1112.0
	1408.0

Impact on Weighted Mean Activity Uncertainties - I

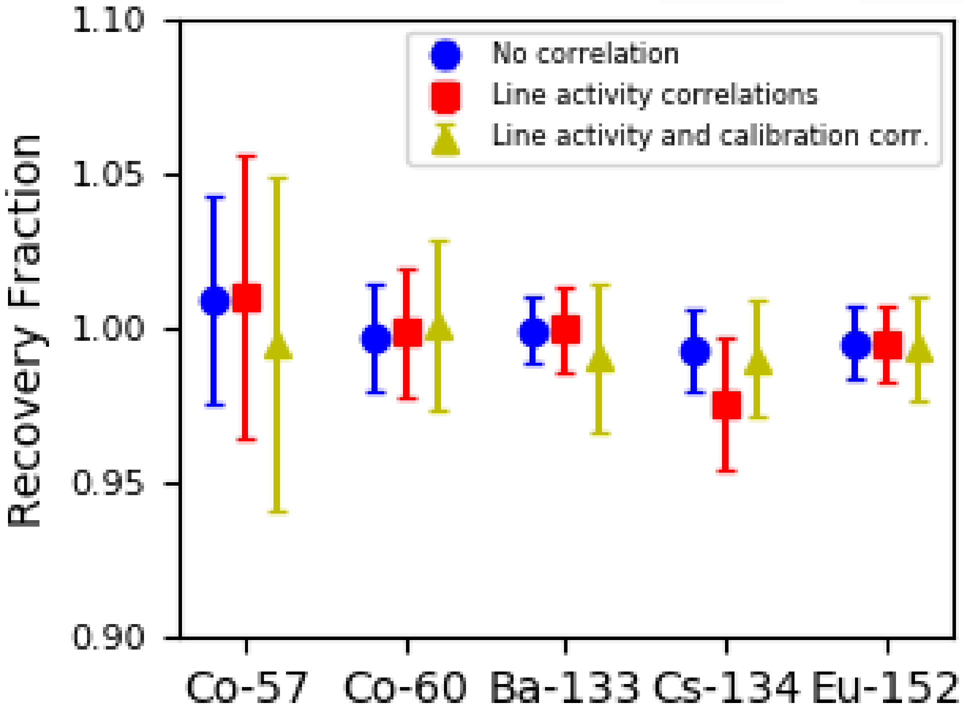
- Mixed Gamma Calibration Standard (minimal correlation)
- "Dual" Efficiency Model
- Changes in reported activities were minimal
- Changes in reported uncertainties were more significant:



Sample Nuclide	No Correlation	Line Activity Correlations Only	Line Activity & Cal. Standard Correlations
CO-57	1.574%	1.991%	1.986%
CO-60	1.275%	1.699%	1.890%
BA-133	1.248%	1.522%	1.501%
CS-134	1.024%	1.603%	1.538%
EU-152	0.685%	1.036%	1.104%

Impact on Weighted Mean Activity Uncertainties - II

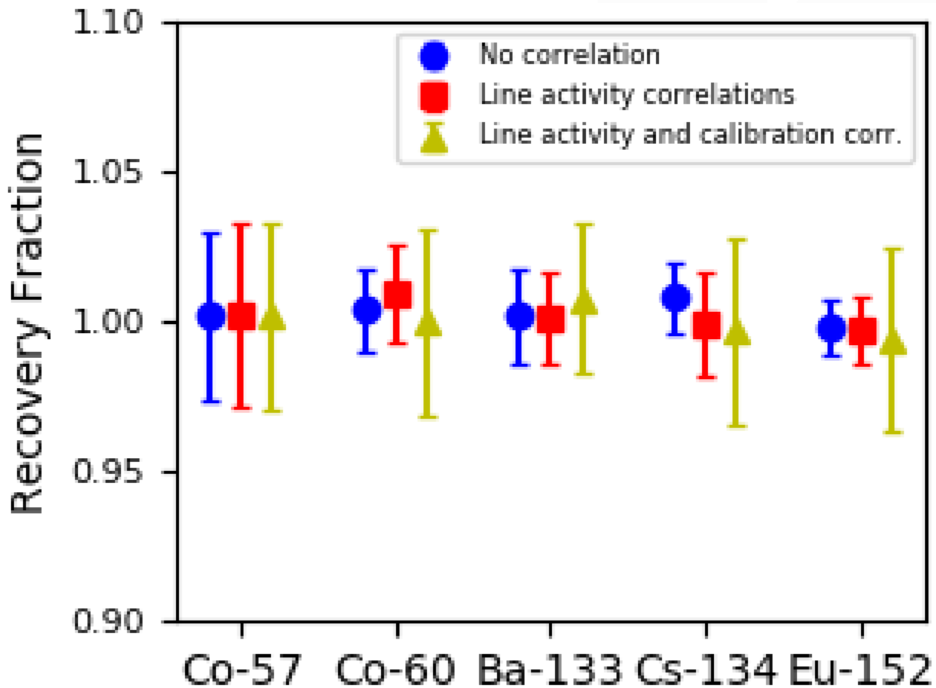
- AmBaCsCo Calibration Standard (moderate correlations)
- Dual Curve (crossover at 276 keV)
- Similar results to previous (activities show minimal change)
- Line activities generally show greater correlation



Sample Nuclide	No correlation	Line Activity Correlations Only	Line Activity & Cal. Standard Correlations
CO-57	3.319%	4.506%	5.425%
CO-60	1.733%	2.105%	2.729%
BA-133	1.081%	1.360%	2.390%
CS-134	1.347%	2.192%	1.869%
EU-152	0.888%	1.232%	1.707%

Impact on Weighted Mean Activity Uncertainties - III

- AmEu Calibration Standard (greatest correlation)
- Linear Efficiency Model
- Similar results to previous (activities show minimal change)
- When Calibration Standard correlations are included, final activity uncertainties > Cal Source Uncertainty (3%) (except Ba-133)



Sample Nuclide	No correlation	Line Activity Correlations Only	Line Activity & Cal. Standard Correlations
CO-57	2.757%	3.039%	3.092%
CO-60	1.349%	1.646%	3.058%
BA-133	1.586%	1.554%	2.450%
CS-134	1.144%	1.719%	3.087%
EU-152	0.756%	1.107%	3.073%

Interference Correction Examples – Testing Approach

- Simulated sample spectra with Se-75, Co-57, and Eu-152 were used to demonstrate the effects of correlations on Interference Correction results
- Both Co-57 lines are shared by other nuclides, so activity quantification/identification relies on interference correction to identify excess counts at 122 & 136 keV

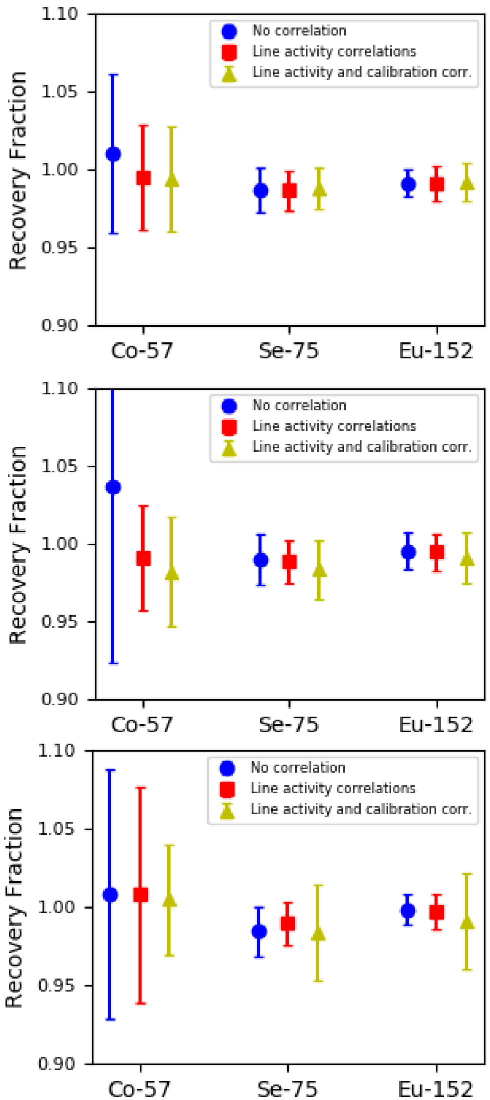
Se-75	Co-57	Eu-152
97		
122	122	122
136	136	
		245
265		
280		
		344
400		
		778
		867
		964
		1086
		1112
		1408

Gamma Energies of Interference Nuclides (keV)

Impact on Interference Correction Uncertainties - Results

- Activity Uncertainties for Interference Correction Nuclides

Calibration Standard	NID Nuclide	No Correlation	NID Correlation Effects	NID & Cal. Std. Correlation effects.
Mixed Gamma	CO-57 SE-75 EU-152	4.992% 1.447% 0.719%	3.378% 1.257% 1.103%	3.36% 1.30% 1.19%
AmBaCsCo	CO-57 SE-75 EU-152	11.586% 1.663% 0.893%	3.359% 1.382% 1.211%	3.49% 1.86% 1.65%
AmEu	CO-57 SE-75 EU-152	7.819% 1.607% 0.770%	6.956% 1.368% 1.133%	3.55% 3.13% 3.09%



Conclusions and where we are today

- The conclusion: approach works well for ideal data sets
- For more challenging “realistic” data sets
  - For example, when the efficiency calibration does not quite match the efficiency response or peak fitting is incorrect
  - Preliminary testing shows the algorithm is extremely sensitive to inconsistencies in the data
  - A peak selection algorithm is being explored to input only the most accurate data into the algorithm
  - Fall back to traditional (non-correlated) algorithm if data is too inconsistent

Conclusions and where we are today

- Enhanced analysis engines in development for Genie 2000 to correctly account for correlations
  - Between measured efficiency calibration data
  - Between nuclide line activities
- Correlations generally have minimal effect on activity values, but could change some single line nuclide results or interference corrected activities by a percent or more in some cases
- Correlations have more impact on correctly defining the activity uncertainty, with changes of several percent in uncertainty for common scenarios
- These effects could be particularly important for high-precision applications
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