ADVANCED SYNTHETICALLY ENHANCED DETECTOR RESOLUTION ALGORITHM: A SYSTEM FOR EXTRACTING PHOTOPEAKS FROM A SODIUM IODIDE SCINTILLATION DETECTOR SPECTRUM

By

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## TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACKNOWLEDGMENTS</td>
<td>3</td>
</tr>
<tr>
<td>LIST OF TABLES</td>
<td>6</td>
</tr>
<tr>
<td>LIST OF FIGURES</td>
<td>7</td>
</tr>
<tr>
<td>ABSTRACT</td>
<td>11</td>
</tr>
<tr>
<td><strong>CHAPTER</strong></td>
<td></td>
</tr>
<tr>
<td>1 INTRODUCTION</td>
<td>12</td>
</tr>
<tr>
<td>2 PREVIOUS WORK</td>
<td>13</td>
</tr>
<tr>
<td>2.1 Gamma Detector Response and Analysis Software (GADRAS)</td>
<td>13</td>
</tr>
<tr>
<td>2.2 Maximum Entropy</td>
<td>13</td>
</tr>
<tr>
<td>2.3 Maximum Likelihood</td>
<td>14</td>
</tr>
<tr>
<td>2.4 New Approach</td>
<td>14</td>
</tr>
<tr>
<td>3 ADAPTIVE SPECTRAL DENOISING BY CHI-SQUARED ANALYSIS</td>
<td>15</td>
</tr>
<tr>
<td>3.1 Smoothing</td>
<td>15</td>
</tr>
<tr>
<td>3.2 Chi-Squared Analysis</td>
<td>17</td>
</tr>
<tr>
<td>3.3 Chi-Processed Denoising Algorithm</td>
<td>18</td>
</tr>
<tr>
<td>3.4 Adaptive Chi-Processed Denoising Algorithm</td>
<td>23</td>
</tr>
<tr>
<td>3.5 Method for Least-Squares Fitting</td>
<td>24</td>
</tr>
<tr>
<td>3.6 Suitability for Real-Time Spectral Analysis</td>
<td>30</td>
</tr>
<tr>
<td>4 GENERATING SYNTHETIC PHOTOPeAKS AND SPECTRA FOR A GAMMA RAY DETECTOR</td>
<td>31</td>
</tr>
<tr>
<td>4.1 Monte Carlo N-Particle Transport (MCNP) Simulations</td>
<td>31</td>
</tr>
<tr>
<td>4.2 Denoising</td>
<td>32</td>
</tr>
<tr>
<td>4.3 Interpolation</td>
<td>32</td>
</tr>
<tr>
<td>4.4 Electronic Broadening</td>
<td>39</td>
</tr>
<tr>
<td>4.5 Complete Detector Spectra</td>
<td>41</td>
</tr>
<tr>
<td>4.6 Applications for Synthetically Generated Detector Response Functions</td>
<td>42</td>
</tr>
<tr>
<td>5 PEAK SEARCH ALGORITHM</td>
<td>43</td>
</tr>
<tr>
<td>5.1 Input Files</td>
<td>45</td>
</tr>
<tr>
<td>5.2 Example</td>
<td>48</td>
</tr>
<tr>
<td>6 PEAK SEARCH WITH SIMULATED SPECTRA AND NO NOISE</td>
<td>62</td>
</tr>
<tr>
<td>6.1 Cesium-137</td>
<td>62</td>
</tr>
<tr>
<td>6.2 Cobalt-60</td>
<td>64</td>
</tr>
</tbody>
</table>
6.3 Barium-133 .................................................. 66

7 PEAK SEARCH WITH SIMULATED SPECTRA AND NOISE ............... 69

7.1 Cesium-137 .................................................. 69
7.2 Cobalt-60 .................................................... 70
7.3 Barium-133 .................................................. 70

8 PEAK SEARCH WITH MEASURED DETECTOR SPECTRA .................... 80

8.1 Cesium-137 .................................................. 80
8.2 Cobalt-60 .................................................... 80
8.3 Barium-133 .................................................. 81
8.4 Plutonium Berillium (PuBe) .................................. 82

9 CONCLUSION ..................................................... 91

9.1 Adaptive Chi-Processed (ACHIP) Denoising .............................. 91
9.2 Detector Response Generation .................................... 91
9.3 Detector Spectrum Deconvolution .................................. 92

10 FUTURE WORK .................................................. 93

10.1 Adaptive Chi-Processed (ACHIP) Denoising .............................. 93
10.2 Detector Response Generation .................................... 93
10.3 Detector Spectrum Deconvolution .................................. 94

APPENDIX

A GRAPHICAL USER INTERFACE .................................. 95

REFERENCES ..................................................... 97

BIOGRAPHICAL SKETCH .......................................... 98
<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-1</td>
<td>Detector response function features.</td>
<td>35</td>
</tr>
<tr>
<td>4-2</td>
<td>Detector resolution (full-width half-max) calibration data.</td>
<td>39</td>
</tr>
<tr>
<td>8-1</td>
<td>Energy calibration data</td>
<td>80</td>
</tr>
</tbody>
</table>
### LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>3-1</td>
<td>Monte Carlo generated detector response function for a 350 keV gamma source and a sodium iodide scintillation detector.</td>
<td>16</td>
</tr>
<tr>
<td>3-2</td>
<td>Weighted averaging applied to a Monte Carlo generated detector response function.</td>
<td>17</td>
</tr>
<tr>
<td>3-3</td>
<td>Chi-processed denoising algorithm algorithm applied to a Monte Carlo generated response function.</td>
<td>20</td>
</tr>
<tr>
<td>3-4</td>
<td>Excerpt from a Ba-133 spectrum, collected with a sodium iodide scintillation detector.</td>
<td>21</td>
</tr>
<tr>
<td>3-5</td>
<td>Chi-processed denoising algorithm applied to a measured Ba-133 spectrum.</td>
<td>21</td>
</tr>
<tr>
<td>3-6</td>
<td>Excerpt from a measured detector spectrum for Ba-133.</td>
<td>22</td>
</tr>
<tr>
<td>3-7</td>
<td>Adaptive chi-processed denoising algorithm applied to a Ba-133 spectrum.</td>
<td>23</td>
</tr>
<tr>
<td>3-8</td>
<td>Adaptive chi-processed denoising algorithm applied to a measured Ba-133 detector response function.</td>
<td>25</td>
</tr>
<tr>
<td>3-9</td>
<td>Monte Carlo generated detector response function for a 350 keV gamma source and a sodium iodide scintillation detector.</td>
<td>26</td>
</tr>
<tr>
<td>3-10</td>
<td>Chi-processed denoising algorithm applied to a Monte Carlo generated detector response function.</td>
<td>27</td>
</tr>
<tr>
<td>3-11</td>
<td>Adaptive chi-processed denoising algorithm applied to a Monte Carlo generated detector response function.</td>
<td>28</td>
</tr>
<tr>
<td>3-12</td>
<td>Monte Carlo generated detector response function for a 350 keV gamma source and a sodium iodide scintillator with fewer histories.</td>
<td>29</td>
</tr>
<tr>
<td>3-13</td>
<td>Adaptive chi-processed denoising algorithm applied to a Monte Carlo generated detector response function with fewer histories.</td>
<td>30</td>
</tr>
<tr>
<td>4-1</td>
<td>Monte Carlo transport model of NaI system with scattering plate.</td>
<td>32</td>
</tr>
<tr>
<td>4-2</td>
<td>Monte Carlo simulation of energy deposited per photon in a NaI(Tl) scintillation detector from a 650 keV source.</td>
<td>33</td>
</tr>
<tr>
<td>4-3</td>
<td>Result of applying the ACHIP denoising tool to the MCNP pulse height tally in Figure 4-2.</td>
<td>34</td>
</tr>
<tr>
<td>4-4</td>
<td>Interpolated response function for a monoenergetic 662 keV source with a 1.4 million count photopeak.</td>
<td>37</td>
</tr>
</tbody>
</table>
4-5 Absolute interpolation error for the interpolated response function in Figure 4-4 when compared to a direct MCNP simulation for a 662 keV source.

4-6 Illustration of low-energy tailing in simulated electronic broadening.

4-7 Simulated detector response for Ba-133, combining detector response functions for eight emission energies.

4-8 Measured detector response spectrum for Ba-133, for comparison with the simulated detector response in Figure 4-7.

5-1 Advanced synthetically enhanced detector resolution algorithm flow diagram.

5-2 Advanced synthetically enhanced detector resolution algorithm settings file, which is always named “process.txt.”

5-3 Detector resolution calibration file.

5-4 Energy calibration file.

5-5 Synthetically generated Ba-133 sample spectrum.

5-6 Remainder spectrum is shown in blue and is identical to the original sample spectrum. The first identified peak is shown in red.

5-7 Original sample spectrum is shown in blue. The remainder spectrum, after subtracting the first identified peak, is shown in red.

5-8 Remainder spectrum is shown in blue. The second identified peak is shown in red.

5-9 Original sample spectrum is shown in blue. The remainder spectrum, after subtracting the first two identified peaks, is shown in red.

5-10 Remainder spectrum is shown in blue. The third identified peak is shown in red.

5-11 Original sample spectrum is shown in blue. The remainder spectrum, after subtracting the first three identified peaks, is shown in red.

5-12 Remainder spectrum is shown in blue. The fourth identified peak is shown in red.

5-13 Original sample spectrum is shown in blue. The remainder spectrum, after subtracting the first four identified peaks, is shown in red.

5-14 Remainder spectrum is shown in blue. The fifth identified peak is shown in red.

5-15 Original sample spectrum is shown in blue. The remainder spectrum, after subtracting the first five identified peaks, is shown in red.

5-16 Remainder spectrum is shown in blue. The sixth identified peak is shown in red.
5-17 Original sample spectrum is shown in blue. The remainder spectrum, after subtracting all six identified peaks, is shown in red. 

6-1 Input file for generating a simulated Cs-137 detector response function. 

6-2 Input settings file for simulated Cs-137. 

6-3 Detector resolution calibration data. 

6-4 Advanced synthetically enhanced detector resolution algorithm results overlayed on the original simulated Cs-137 detector response function. 

6-5 Input file for generating a simulated Co-60 detector response function. 

6-6 Advanced synthetically enhanced detector resolution algorithm (ASEDRA) results overlayed on the original simulated Co-60 detector response function. ASEDRA found both peaks: 1173 keV and 1332 keV. 

6-7 Input file for generating a simulated Ba-133 detector response function. 

6-8 Advanced synthetically enhanced detector resolution algorithm (ASEDRA) results overlayed on the original simulated Ba-133 detector response function. ASEDRA found all of the photopeaks, including the overlapping peaks at 276/303 keV and 356/384 keV. 

7-1 Adaptive denoising is turned on by setting the chi-squared threshold to -1. All other settings are identical to the settings in the previous chapter. 

7-2 Simulated, one-minute, Cs-137 detector response function with Poisson noise. 

7-3 Advanced synthetically enhanced detector resolution algorithm (ASEDRA) results overlayed on the denoised version of the simulated Cs-137 detector response function in Figure 7-2. ASEDRA found the only photopeak at 661 keV. 

7-4 Simulated, one-minute, Co-60 detector response function with Poisson noise. 

7-5 Advanced synthetically enhanced detector resolution algorithm (ASEDRA) results overlayed on the denoised version of the simulated Co-60 detector response function in Figure 7-4. ASEDRA found both photopeaks at 1176 keV and 1336 keV. 

7-6 Simulated, one-minute, Ba-133 detector response function with Poisson noise. 

7-7 Advanced synthetically enhanced detector resolution algorithm results overlayed on the denoised version of the simulated, one-minute Ba-133 detector response function in Figure 7-6. 

7-8 Advanced synthetically enhanced detector resolution algorithm results for the simulated, one-minute Ba-133 detector response function in Figure 7-6. Denoising was not used for these results.
7-9  Simulated, five-minute, Ba-133 detector response function with Poisson noise.

7-10  Advanced synthetically enhanced detector resolution algorithm results overlayed on the denoised version of the simulated Ba-133 detector response function in Figure 7-9.

7-11  Advanced synthetically enhanced detector resolution algorithm results for the simulated, five-minute Ba-133 detector response function in Figure 7-9. Denoising was not used for these results.

8-1  Measured, one-minute, Cs-137 detector response function.

8-2  Advanced synthetically enhanced detector resolution algorithm results overlayed on the denoised version of the measured, one-minute Cs-137 detector response function in Figure 8-1.

8-3  Measured, one-minute, Co-60 detector response function.

8-4  Advanced synthetically enhanced detector resolution algorithm results overlayed on the denoised version of the measured, one-minute Co-60 detector response function in Figure 8-3.

8-5  Measured, one-minute, Ba-133 detector response function.

8-6  Advanced synthetically enhanced detector resolution algorithm results overlayed on the denoised version of the measured, one-minute Ba-133 detector response function in Figure 8-5.

8-7  Measured, one-minute, PuBe detector response function.

8-8  Advanced synthetically enhanced detector resolution algorithm results overlayed on the denoised version of the measured, one-minute PuBe detector response function in Figure 8-7.

8-9  Advanced synthetically enhanced detector resolution algorithm results from Figure 8-8 compared with a denoised, higher resolution (Germanium) spectrum for the same sample.

8-10 Advanced synthetically enhanced detector resolution algorithm results for a simulated PuBe spectrum with no stochastic noise.

A-1  A graphic user interface for ASEDRA is available as an alternative to editing the process.txt file.
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There is a growing demand for low cost, portable (room temperature), high resolution gamma-ray detector systems. Sodium iodide scintillators meet most of these requirements, but do not provide sufficient energy resolution.

I have developed a novel algorithm for spectral deconvolution of sodium iodide scintillation detector spectra. My adaptive chi-processed (ACHIP) denoising algorithm removes the results of stochastic noise from low-count detector spectra. Photopeaks are rapidly identified, starting at the high-energy end of the spectrum. I estimate the detector response functions for photopeaks with a combination of Monte Carlo simulations and simple transformations. The advanced synthetically enhanced detector resolution algorithm (ASEDRA) has a very simple method for identifying photopeaks, based on recognizing local maxima in a detector spectrum. For each identified photopeak, a corresponding detector response function is subtracted from the detector spectrum, revealing previously hidden photopeaks so that highly overlapping photopeaks can be separated. Despite its simplicity, ASEDRA has a demonstrated capability for deconvolving intricate detector spectra.
CHAPTER 1
INTRODUCTION

Roughly half of all sea-borne containers entering the U.S. in May 2006 were screened for radiological weapons and materials [1]. Portal monitoring is an enormous task, requiring accurate nuclide identification. Costs per portal monitoring system must be low enough to provide inspections at each entry point to the United States, and analysis of results must be fast enough to keep traffic moving.

There is a growing demand for low cost, portable (room temperature), high resolution gamma-ray detector systems. Sodium iodide (NaI) scintillators meet most of these requirements, but do not provide sufficient energy resolution. There have been many approaches investigated for post-processing of NaI scintillator output for synthetically enhanced resolution.

I have developed a novel algorithm for spectral deconvolution of NaI scintillator output. Using a combination of previously developed methodologies, novel processing schemes, and radiation simulation data, the advanced synthetically enhanced detector resolution algorithm (ASEDRA) synthetically enhances the resolution of a poor resolution spectrum collected from a sodium iodide (NaI) detector-photomultiplier system. In fact, the algorithm can synthetically extract enhanced doublets from unresolved, low resolution peaks. This new computer algorithm, implemented as a spectral post-processing code, rapidly processes the collected spectrum and synthetically renders photopeaks based on a specific set of parametric peak search criteria.

The photopeak search capability of ASEDRA is built on a foundation of more specific tools, including the adaptive chi-processed (ACHIP) denoising algorithm and a detector response function generator. I discuss the photopeak search algorithm and its capabilities, as well as ideas for further development of the ASEDRA algorithm.
Spectral deconvolution for NaI(Tl) scintillation detectors is a fifty-year-old problem. While NaI detectors are rugged, portable, relatively inexpensive, and have high detection efficiencies, their poor energy resolution complicates photopeak identification. Gamma detector response and analysis software (GADRAS) [2, 3] is currently the industry leader for nuclide identification, and a variety of other methods [4, 5] have been developed for resolution enhancement in support of photopeak identification.

2.1 Gamma Detector Response and Analysis Software (GADRAS)

GADRAS follows a very different strategy than the other methods described in this chapter. GADRAS matches the detector with a parameterized template, then uses that model to construct a voluminous library of nuclide detector response functions. GADRAS then tries to represent the measured spectrum as a linear combination of nuclides and shielding effects from its library.

The advanced synthetically enhanced detector resolution algorithm (ASEDRA) uses a detector model that is based on Monte Carlo N-particle transport (MCNP) [6] simulation, rather than on a parameterized template as in GADRAS. ASEDRA also analyzes detector spectra, without any knowledge of common nuclides, to identify and characterize photopeaks. One advantage of ASEDRA’s approach, which relies on local analysis rather than global analysis, is that interference in one part of the spectrum should not prevent ASEDRA from correctly identifying photopeaks in another part of the spectrum. After ASEDRA identifies the photopeaks in a detector spectrum, another tool can be used to correlate those photopeaks with specific nuclides.

2.2 Maximum Entropy

The maximum entropy method enhances the resolution of a detector spectrum by maximizing Equation 2–1, in which $S$ is a measure of entropy, as defined in Equation 2–2, and $\lambda$ is the smoothing/regularizing term. The functions $f$ and $m$ represent the enhanced
and measured detector responses, respectively, while \( f_j \) and \( m_j \) represented the values of those functions at channel \( j \) in a detector with \( N \) channels.

\[
L(f, \lambda) = \lambda S(f, m) - \frac{1}{2} \chi^2
\]  

(2-1)

\[
S(f, m) = \sum_{j=1}^{N} f_j - m_j - f_j \log \frac{f_j}{m_j}
\]  

(2-2)

The maximum entropy, as well as the maximum likelihood method that is described next, involve iterative convergence, and therefore require significant computation time [5].

### 2.3 Maximum Likelihood

The maximum likelihood method follows the iteration rule shown in Equation 2–3. \( I \) is an estimate of the incident radiation spectrum, and \( m \) is the measured absorption spectrum. \( R \) is a response function matrix, which maps incident source energies to measured responses in channels.

\[
I_{new}(j) = I_{old}(j) \sum_{i=1}^{M} \frac{m(i) R_{ij}}{\sum_{j=1}^{N} I_{old}(j) R_{ij}}
\]  

(2–3)

While the maximum likelihood method does an excellent job at identifying and characterizing photopeaks, this method is also very computationally intensive [5].

### 2.4 New Approach

The advanced synthetically enhanced detector resolution algorithm (ASEDRA) analyzes detector spectra based on the actual physics and a simple heuristic algorithm, without using any information about nuclides of interest. Additionally, ASEDRA provides very fast spectral post-processing, suitable for real-time applications.
CHAPTER 3
ADAPTIVE SPECTRAL DENOISING BY CHI-SQUARED ANALYSIS

The advanced synthetically enhanced detector resolution algorithm (ASEDRA) was designed for real-time applications. In addition to software execution time, it is important to remember that the time available for radiation measurement is also limited.

Time constraints often prevent us from taking thorough radiation measurements. In a portal screening system, short count times are necessary to avoid delaying traffic. When the number of counts per channel is too low, stochastic noise becomes problematic. Filtering white noise from spectral data, while preserving sharp peaks, is useful for visualization of noisy spectra, or as a preprocessing step for spectral analysis algorithms. I developed an algorithm \cite{7, 8} that addresses this noise reduction need while minimizing the degradation of sharp features of interest in the spectrum; the algorithm is summarized here. In this chapter, I discuss smoothing and denoising techniques for Monte Carlo simulated \cite{6} and actual radiation detector spectral data, focusing in particular on a new algorithm based on chi-squared analysis.

3.1 Smoothing

Spectral data denoising is essential to enhance radiation counting pulse height data collected using a detector and multi-channel analyzer system. Random variation in counts per channel, leading to jagged edges in spectral data, can be readily filtered by weighted averaging or polynomial fitting. Equation 3–1, for example, implements a form of weighted averaging which is commonly used for gamma detector spectra \cite{9}. $F(x)$ represents the spectrum after smoothing, while $f(x)$ represents the original measured spectrum.

\[
F(x) = \frac{3}{8} f(x) + \frac{1}{4} f(x - 1) + \frac{1}{4} f(x + 1) + \frac{1}{16} f(x - 2) + \frac{1}{16} f(x + 2)
\]

(3–1)

The weighted averaging process, however, may broaden or remove real features of interest from the spectrum. Figure 3-1 shows an MCNP-generated detector response
function with several real, sharp features, as well as noticeable stochastic noise. Figure 3-2 shows the same detector response function after applying the weighted averaging technique for smoothing. The two x-ray escape peaks around 320 keV are so broadened that they are no longer distinguishable after smoothing. The K-shell edge around 40 keV, while still visible, is also broadened and reduced in prominence.

Figure 3-1. A Monte Carlo generated detector response function for a 350 keV gamma source and a sodium iodide scintillator with 1.2x10^9 histories (plotted as counts vs deposited γ-ray energy). Pulse height tallies are sharper than experimental spectra because electronic broadening is not simulated.

My approach is to distinguish noisy regions, in which stochastic fluctuation dominates and smoothing is essential, from regions with sharp, statistically significant features, in which smoothing attempts may be destructive. This determination is based on a common technique from statistics: chi-squared analysis.
Figure 3-2. After applying weighted averaging to the Monte Carlo generated detector response function in Figure 3-1, the stochastic noise is significantly reduced. The two sharp features around 320 keV, however, can no longer be resolved. The K-shell discontinuity around 40 keV, while still visible, is broadened and reduced in prominence.

3.2 Chi-Squared Analysis

Chi-squared analysis is a standard technique for determining how well a given model fits a data set. In particular, I am interested in whether there is a statistically significant difference in counts between two neighboring channels: \( A \) and \( B \). \( N \), in Equation 3-2, is the sum of \( n_A \) and \( n_B \), the counts accumulated in channels \( A \) and \( B \) respectively.

\[
X^2 = \frac{(n_A - N/2)^2}{N/2} + \frac{(n_B - N/2)^2}{N/2} \quad (3-2)
\]
$\chi^2$ is a measure of certainty that the difference between $n_A$ and $n_B$ is due to a difference in expected value, rather than the result of stochastic fluctuation. A $\chi^2$ value of 7.88, when there is one degree of freedom as in Equation 3–2, corresponds to a certainty of 99.5% [10], indicating that this difference in neighboring channels is a statistically significant feature. In the context of gamma detector spectra, such features should be preserved. For lower values of $\chi^2$, the difference is attributable to stochastic fluctuation and should be smoothed away. Chi-squared analysis is traditionally parameterized by $\alpha$, which is the probability that the test incorrectly indicates a significant difference. In this case, $\alpha = 1 - 0.995 = 0.005$.

### 3.3 Chi-Processed Denoising Algorithm

As discussed in the previous section, I identify a set of noise-dominated regions, in which $\chi^2 < 7.88$ for all adjacent channels. The chi-processed denoising algorithm (CHIP) performs smoothing only within these noise-dominated regions, thus guaranteeing that statistically significant features will be preserved.

Within each noise-dominated region, CHIP provides smoothing via a sequence of best-fit lines of the form in Equation 3–3.

$$F(x) = mx + b \quad (3–3)$$

For a given channel $x_o$, I choose parameters $m$ and $b$ (representing slope and intercept) so that $F(x)$ provides the best possible model for the five closest channels (excluding any channels outside the noise-dominated region). To determine how well a given model fits the measured data, I again turn to chi-squared analysis, as in Equation 3–4.
\[
X^2 = \sum_i \frac{(n_i - E(n_i))^2}{E(n_i)}
\]

\[
= \sum_{i=-2}^{2} \frac{(f(x_o + i) - F(x_o + i))^2}{F(x_o + i)}
\]

\[
= \sum_{i=-2}^{2} \frac{(f(x_o + i) - m(x_o + i) - b)^2}{m(x_o + i) + b}
\]

By minimizing \(X^2\), I identify a model \(F(x)\) which matches, as well as possible, a neighborhood of five points around \(x_o\): \(\{x_o - 2, x_o - 1, x_o, x_o + 1, x_o + 2\}\). Then I use that model to choose a new value at \(x_o\).

The CHIP algorithm performs much better than weighted averaging on the example shown in Figure 3-1. The effect of the CHIP algorithm is shown in Figure 3-3. Compared with weighted averaging in Figure 3-2, CHIP provides similar smoothing quality in those areas that need it. The advantage of CHIP, however, is that it does not degrade the spectrum in those areas where smoothing is harmful. The two x-ray escape peaks around 320 keV, for example, are left untouched, as is the K-edge discontinuity around 40 keV.

The second example, in Figure 3-4, shows an excerpt from a Ba-133 spectrum, collected with a sodium iodide scintillation detector.

The CHIP denoising algorithm provides significant reduction of stochastic fluctuation for a measured Ba-133 spectrum, as shown in Figure 3-5, while still preserving significant features. The small full-energy photopeak at 276 keV, for example, remains visible while nearby stochastic noise is removed. Unfortunately, denoising is not sufficient to resolve the convoluted peak at 384 keV, which is roughly seven times smaller than the nearby peak at 356 keV.

These results clearly demonstrate that the CHIP algorithm, applied to radiation detector data, can significantly reduce stochastic noise in a gamma detector spectrum, while preserving statistically significant features.
Figure 3-3. Chi-processed denoising algorithm applied to a Monte Carlo generated response function with $1.2 \times 10^9$ histories. Compare with the original measured spectrum in Figure 3-1.

The CHIP algorithm is far from perfect, however. The stochastic noise is not completely removed in any of these examples and, as shown in Figures 3-6 and 3-7, the algorithm can even introduce defects into a spectrum.

The CHIP algorithm determines that stochastic noise is an issue in Figure 3-6, so that smoothing is needed. Unfortunately, CHIP smoothing is based on linear fitting over a neighborhood of five channels. This does not work well in regions with significant curvature, and Figure 3-7 shows the result. The problem is that the CHIP algorithm uses an assumption that locally constant, over a neighborhood of two channels, implies locally linear, over a larger neighborhood of five channels. Therefore, small noisy regions
Figure 3-4. Excerpt from a Ba-133 spectrum, collected with a sodium iodide scintillation detector.

Figure 3-5. The chi-processed denoising algorithm applied to the measured Ba-133 spectrum in Figure 3-4.
Figure 3-6. Excerpt from a measured detector spectrum for Ba-133.

of a spectrum are linearized without regard for any curvature in the original measured spectrum.

One possible solution to this problem is to fit parabolas, which can better represent curved regions, rather than lines. Another issue is the amount of noise reduction. Fitting over a larger number of points (rather than just five channels) would increase the degree of noise reduction, but choosing too many points could cause problems when a parabola is unable to adequately represent the entire region. Based on experience with my first denoising algorithm, CHIP, I created the adaptive chi-processed denoising (ACHIP) algorithm, which combines parabolic fitting with dynamic range selection to address all of these issues.
Figure 3-7. Result of applying the chi-processed denoising algorithm to the Ba-133 spectrum in Figure 3-6. The incorrect assumption that local linearity over a region of five channels is implied by local constancy over each pair of neighboring channels leads to a “chopping” defect.

3.4 Adaptive Chi-Processed Denoising Algorithm

The CHIP algorithm, discussed in Section 3.3, uses a two-step process, in which it first determines whether smoothing is necessary in some region, and then performs the smoothing operation. The adaptive chi-processed denoising algorithm (ACHIP) follows a more sophisticated approach, in which the smoothing process is adapted to each situation. The ACHIP algorithm uses as many channels as possible, increasing the power of the smoothing operation, within the constraint that the fitted model must match the measured data according to chi-squared analysis. ACHIP also fits parabolic models, rather
than linear models, to increase the number of channels that can reasonably be used in regions with high curvature.

In order to determine a new, denoised value for some channel \( x_o \), ACHIP starts by considering a neighborhood of three channels around \( x_o \). A parabolic model can be chosen to exactly match those three points. Additional channels are added one-by-one, as long as a parabolic model can be found that adequately represents the expanded range, according to a chi-squared test with a 99.5% threshold. Parabolic models are selected by least-square fitting for the sake of faster calculation, as described in Section 3.5, but a model is rejected if chi-squared analysis shows with 99.5% certainty that the model does not adequately represent the experimental data. In other words, the ACHIP algorithm will tend to smooth away features unless there is 99.5% certainty that those features are not the result of stochastic noise. By choosing as many points as possible for each parabolic fitting, the effects of stochastic noise are minimized.

The process of adding additional channels continues until it is no longer possible to further increase the size of the neighborhood while still passing the chi-squared test. This final model then predicts an appropriate denoised value for the channel of interest, \( x_o \).

### 3.5 Method for Least-Squares Fitting

The adaptive chi-processed (ACHIP) denoising algorithm requires fitting of parabolic models to a set of measured data points. This fitting process is the most computationally demanding step in the ACHIP algorithm, and fast execution is essential for real-time denoising of field measurements. In this section I describe a fast method for determining parabolic least-square fits.

Suppose I need to fit a parabola over a set of \( N \) evenly separated channels. I can represent the measured data as \( \vec{m} = (m_1, m_2, \cdots m_N) \). A parabola is any function of the form \( f(x) = c_0 + c_1 x + c_2 x^2 \), so I could also define a set of vectors, \( \{\vec{v}_0, \vec{v}_1, \vec{v}_2\} \), representing \( \{1, x, x^2\} \), as in Equation 3–5.
Figure 3-8. Adaptive chi-processed denoising algorithm removes noise from the spectrum in Figure 3-6 without introducing defects. Compare with Figure 3-7 in which chi-processed denoising algorithm actually made this spectrum worse.

\[ \vec{v}_0 = (1, 1, \cdots 1) \]
\[ \vec{v}_1 = (1, 2, \cdots N) \]
\[ \vec{v}_2 = (1^2, 2^2, \cdots N^2) \]

(3–5)

A parabola vector \( \vec{u} \) could then be defined as in Equation 3–6.

\[ \vec{u} = c_0 \vec{v}_0 + c_1 \vec{v}_1 + c_2 \vec{v}_2 \]

(3–6)
Figure 3-9. Monte Carlo generated detector response function for a 350 keV gamma source and a sodium iodide scintillator with 1.2x10^8 histories (plotted as counts vs deposited γ-ray energy). Pulse height tallies appear differently from experimental spectra because electronic broadening is not simulated.

The goal is to choose the set of constants \( \{c_0, c_1, c_2\} \) so that \( \bar{u} \) and \( \bar{m} \) will be as close as possible according to the least-squares metric in Equation 3–7.

\[
\sum_{i=1}^{N} (u_i - m_i)^2
\]  \hspace{1cm} (3–7)

It should be clear by inspection that this is equivalent to minimizing the Euclidean difference as shown in Equation 3–9 because, for \( x > 0 \), \( \sqrt{x} \) is a strictly increasing function.
Figure 3-10. Chi-processed denoising algorithm removes some of the noise from the Monte Carlo generated detector response function in Figure 3-9.

\[ < \vec{x}, \vec{y} > = \sum_{i=1}^{N} (x_i - y_i)^2 \] (3–8)

Therefore, I define the dot product as in Equation 3–8 and say that the goal of least-squares fitting is equivalent to minimizing the length \([11]\) of the difference between \(\vec{u}\) and \(\vec{m}\) as in Equation 3–9.

\[ ||\vec{u} - \vec{m}|| = \sqrt{< \vec{u} - \vec{m}, \vec{u} - \vec{m} >} \]

\[ = \sqrt{ \sum_{i=1}^{N} (u_i - m_i)^2 } \] (3–9)
Figure 3-11. Adaptive chi-processed denoising algorithm enhances the Monte Carlo generated detector response function in Figure 3-9. ACHIP produces a much cleaner spectrum than CHIP (compare with Figure 3-10) while still preserving real features.

Determining the value of $\vec{u}$ that minimizes Equation 3–9 would be computationally easier if $\vec{u}$ were expressed as a linear combination of orthonormal vectors. In fact, it is possible to choose a set of orthonormal vectors $\{\vec{w}_0, \vec{w}_1, \vec{w}_2\}$ such that the set of all possible linear combinations of $\{\vec{w}_0, \vec{w}_1, \vec{w}_2\}$ is equivalent to the set of all possible linear combinations of $\{\vec{v}_0, \vec{v}_1, \vec{v}_2\}$. Gram-Schmidt orthogonalization [12] is a standard technique for choosing a set of orthonormal vectors $\{\vec{v}_0, \vec{v}_1, \vec{v}_2\}$ that meet that requirement, as shown in Equation 3–10, in which the dot product and length are defined as in Equations 3–8 and 3–9. An arbitrary parabola $\vec{u}$ can then be represented as $\vec{u} = d_0 \vec{w}_0 + d_1 \vec{w}_1 + d_2 \vec{w}_2$ for some set of constants $\{d_0, d_1, d_2\}$.
Figure 3-12. A Monte Carlo generated detector response function for a 350 keV gamma source and a sodium iodide scintillator with $1.2 \times 10^7$ histories (plotted as counts vs deposited $\gamma$-ray energy). Pulse height tallies appear differently from experimental spectra because electronic broadening is not simulated.

$$\vec{w}_0 = \frac{\vec{v}_0}{||\vec{v}_0||}$$

$$\vec{x}_1 = \vec{v}_1 - \langle \vec{v}_1, \vec{w}_0 \rangle \vec{w}_0$$

$$\vec{w}_1 = \frac{\vec{x}_1}{||\vec{x}_1||}$$

$$\vec{x}_2 = \vec{v}_2 - \langle \vec{v}_2, \vec{w}_0 \rangle \vec{w}_0 - \langle \vec{v}_2, \vec{w}_1 \rangle \vec{w}_1$$

$$\vec{w}_2 = \frac{\vec{x}_2}{||\vec{x}_2||}$$

(3–10)
Figure 3-13. Adaptive chi-processed denoising algorithm enhances the Monte Carlo generated detector response function in Figure 3-12. This is a particularly challenging spectrum, due to the low number of counts in many of the channels. Note that chi-squared analysis does not work well with fewer than 20 counts per channel.

Once the orthonormal vectors \( \{ \vec{w}_0, \vec{w}_1, \vec{w}_2 \} \) are calculated, as described above, the optimal values \( \{ d_0, d_1, d_2 \} \) are easily calculated by \( d_i = \langle \bar{m}, \vec{w}_i \rangle \) [13]. This method is fast because the orthonormal set \( \{ \vec{w}_0, \vec{w}_1, \vec{w}_2 \} \) depends only on the number of channels being considered, and can therefore be reused each time a least squares fitting is performed.

3.6 Suitability for Real-Time Spectral Analysis

The adaptive chi-processed (ACHIP) denoising algorithm greatly reduces the need for long measurement times by removing the effects of stochastic noise. Additionally, the ACHIP algorithm can process a detector spectrum in less than a second.
In order to deconvolute detector spectra into their component photopeaks, it is useful to fully characterize these photopeaks, as well as their associated effects such as Compton edges, x-ray escape peaks, k-edges, and backscatter peaks. I discuss a method for generating full detector response functions, each of which represents the response of a gamma ray detector to a monoenergetic photon source. Such detector response functions can be combined to form complete detector spectra or used individually as part of a spectral deconvolution algorithm.

### 4.1 Monte Carlo N-Particle Transport (MCNP) Simulations

In order to determine how a detector will respond to an x-ray source, such as a radioactive isotope, the first step is to determine how much energy will be deposited in the detector by each source photon. The energy deposited can be determined from pulse height tallies in the MCNP \cite{mcnp} radiation simulation program.

Figure 4-1 shows the MCNP model corresponding to our NaI scintillation detector setup. The sample is represented by a point source, 10.5 cm from the 5 cm square cylindrical NaI(Tl) detector crystal. I performed simulations at a variety of source energies, as well as both with and without a 0.5 cm thick iron plate placed between the source and the detector.

Figure 4-2 shows a histogram of the amount of energy deposited in the detector crystal for each Monte Carlo simulated 650 keV photon. This plot has much sharper features than a real NaI scintillation detector spectrum because it does not include the effects of electronic broadening.

The simulation results in Figure 4-2 required $1.2 \times 10^9$ trials and about 10 hours of computer time. In order to simulate detector responses for radioactive isotopes, such results are needed for a wide variety of source energies from 20 keV up to 3000 keV, leading to enormous amounts of computer time. We used two techniques to reduce the
time requirements for radiation simulation: denoising and interpolation. Denoising reduces the number of trials required for each simulation, and interpolation reduces the number of simulations required.

4.2 Denoising

Like all Monte Carlo results, the data shown in Figure 4-2 are random variables. The accuracy of these values can be improved by increasing the number of trials, but this strategy is computationally expensive. The denoising tool discussed in Chapter 3 provides similar results with much lower computational cost. Figure 4-3 shows the result of only a few additional seconds of processing time with the adaptive chi-processed (ACHIP) denoising algorithm, compared to the original data in Figure 4-2 which took ten hours to generate.

4.3 Interpolation

As part of the advanced synthetically enhanced detector response algorithm (ASE-DRA) peak search capability, we needed to generate detector response functions for
Monte Carlo simulation of energy deposited per photon in a NaI(Tl) scintillation detector from a 650 keV source. The full energy photopeak at 650 keV has a height of $1.45 \times 10^6$ counts. A total of $1.2 \times 10^9$ photons were simulated, many of which did not reach the detector. The iron plate was not included in this simulation.

Figure 4-2. Monte Carlo simulation of energy deposited per photon in a NaI(Tl) scintillation detector from a 650 keV source. The full energy photopeak at 650 keV has a height of $1.45 \times 10^6$ counts. A total of $1.2 \times 10^9$ photons were simulated, many of which did not reach the detector. The iron plate was not included in this simulation.

Monoenergetic sources ranging from 20 keV to 3000 keV. Within the ASEDRA code, we needed the ability to choose source energies to within 1 keV. Simulating so many sources directly in MCNP would be impractical due to time constraints. Therefore, we decided to choose source energies at 50 keV intervals (a factor of 50 reduction in computer time) and estimate response functions for intermediate energies by interpolation. Using interpolation to reduce the computational cost of producing detector response functions is discussed further in section II.B of Meng and Ramsden [5], which in turn cites Kiziah and Lowell [14].
Accurate interpolation between response functions requires transforming those response functions so that their features line up with features in the interpolated response function. Key features in the detector response functions include: the photopeak, single and double escape peaks, the k-edge discontinuity (not considered), the backscatter peak, and the Compton edge. These features change position as a function of source energy, as shown in Equation 4–1. It makes sense, then, to stretch each of the simulated response functions such that the known positions of such features line up with the known positions of the same features in the interpolated response function.
\[ E_{\text{photopeak}} = E_{\text{source}} \]

\[ E_{\text{single-escape}} = E_{\text{source}} - 511 \text{ keV (if } E_{\text{source}} > 1022 \text{ keV)} \]

\[ E_{\text{double-escape}} = E_{\text{source}} - 1022 \text{ keV (if } E_{\text{source}} > 1022 \text{ keV)} \]  \hspace{1cm} (4-1)

\[ E_{\text{backscatter}} = \frac{511 \text{ keV}}{2 + \frac{511 \text{ keV}}{E_{\text{source}}}} \]

\[ E_{\text{Compton}} = E_{\text{source}} - E_{\text{backscatter}} \]

As an example, suppose that MCNP simulations have been performed for photon sources of 300 keV and 350 keV, yielding detector response functions \( f_{300}(E) \) and \( f_{350}(E) \), respectively. A simulation for a source of 310 keV is not available, but an estimate for \( f_{310}(145 \text{ keV}) \) is needed. The first step for estimating \( f_{310}(145 \text{ keV}) \) is to characterize known features of the three response functions, as in Table 4-1.

**Table 4-1. Detector response function features.**

<table>
<thead>
<tr>
<th>Feature</th>
<th>( f_{300} )</th>
<th>( f_{310} )</th>
<th>( f_{350} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Photopeak</td>
<td>300</td>
<td>310</td>
<td>350</td>
</tr>
<tr>
<td>Single escape</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Double escape</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Compton edge</td>
<td>162</td>
<td>170</td>
<td>202</td>
</tr>
<tr>
<td>Backscatter peak</td>
<td>138</td>
<td>140</td>
<td>148</td>
</tr>
<tr>
<td>Zero</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

On the \( f_{310} \) response function, 145 keV is between the backscatter peak at 140 keV and the Compton edge at 170 keV. More precisely, 145 keV is one-sixth of the way from the backscatter peak at 140 keV to the Compton edge at 170 keV. Similarly, 142 keV and 157 keV are one-sixth of the way from the backscatter peak to the Compton edge on the \( f_{300} \) and \( f_{350} \) response functions, respectively. Therefore, \( f_{310}(145 \text{ keV}) \) can be estimated by linear interpolation between \( f_{300}(142 \text{ keV}) \) and \( f_{350}(157 \text{ keV}) \) as in Equation 4–2.
\[ f_{310}(145 \text{ keV}) = \left( \frac{f_{350}(157 \text{ keV}) - f_{300}(142 \text{ keV})}{350\text{keV} - 300\text{keV}} \right) (310\text{keV} - 300\text{keV}) \]
\[ + f_{300}(142 \text{ keV}) \]  
\hspace{1cm} (4-2)

ASEDRA’s interpolation method is actually a simplification of the method described in the previous paragraph and in Equation 4–2. This simplification leads to a reduction in interpolation accuracy, but is more easily implemented and probably runs faster. Instead of noting, for the \( f_{310} \) response function, that that 145 keV is one-sixth of the way from the backscatter peak at 140 keV to the Compton edge at 170 keV, ASEDRA notes that 145 keV is 25 keV less than the Compton edge at 170 keV. Similarly, 137 keV and 177 keV are 25 keV less than the \( f_{300} \) and \( f_{350} \) Compton edges, respectively. Therefore, \( f_{310}(145 \text{ keV}) \) can be estimated by linear interpolation between \( f_{300}(137 \text{ keV}) \) and \( f_{350}(177 \text{ keV}) \) as in Equation 4–3.

\[ f_{310}(145 \text{ keV}) = \left( \frac{f_{350}(177 \text{ keV}) - f_{300}(137 \text{ keV})}{350\text{keV} - 300\text{keV}} \right) (310\text{keV} - 300\text{keV}) \]
\[ + f_{300}(137 \text{ keV}) \]  
\hspace{1cm} (4–3)

This simpler interpolation method gives similar results to the earlier, more accurate interpolation method when estimating the value for an energy which is close to a higher-energy feature. In the example, however, the value of \( f_{310} \) is estimated at 145 keV, which is very close to a lower-energy feature, the backscatter peak at 140 keV. Note that Equation 4–3 suggests that \( f_{310}(145 \text{ keV}) \), which is between the backscatter peak and the Compton edge, is similar to \( f_{300}(137 \text{ keV}) \), which is at a lower energy than the backscatter peak.

ASEDRA’s interpolation method works well for the 662 keV response function shown in Figure 4-4. Figure 4-5 shows the absolute error between that interpolated response function and a direct MCNP simulation for the same energy. Note that the largest absolute errors occur around sharp features in the spectrum: the photopeak, the x-ray
escape peaks, and the Compton edge. The Compton edge in the interpolated spectrum is shifted by 1 keV in the high-energy direction because the interpolation method does not guarantee synchronization on the high-energy side of a feature. The detector has a FWHM of around 40 keV at this energy, so a large error in one channel near the Compton edge only has around a 1% effect on any channel after electronic broadening is considered. The error of 2000 counts at the photopeak is negligible compared to the 1.4 million counts in the photopeak. The Compton continuum has a far more significant error of around 3%, which can be attributed to nonlinearity in the NaI cross sections.

While it may be possible to slightly reduce interpolation error with a more sophisticated algorithm, significant reduction of interpolation error would probably require direct
Figure 4-5. Absolute interpolation error for the interpolated response function in Figure 4-4 when compared to a direct MCNP simulation for a 662 keV source. Simulation of more source energies. One possibility is to perform direct simulation of “interesting” source energies, such as the photopeak energies for nuclides of interest, to supplement the equally spaced source energies that have already been simulated. Another possibility is to perform simulations at a much larger number of source energies, but with fewer histories per simulation, and deal with the resulting stochastic noise by applying a 2-D denoising algorithm to the entire library of detector response functions. Such a strategy would increase accuracy by completely eliminating the need for interpolation.
4.4 Electronic Broadening

The effect of electronic broadening on detector response functions can be approximated by a Gaussian transformation. The Gaussian distribution is defined in Equation 4–4. The Gaussian transformation is defined in Equation 4–5 and transforms counts $C_{\text{old}}$ as a function of energy in a pulse height tally to counts $C_{\text{new}}$ as a function of energy in a realistic detector response function.

$$G(x; \mu, \sigma) = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}, \text{ where } \sigma = \text{FWHM}/2.35$$  \hspace{1cm} (4–4)

$$C_{\text{new}}(x) = \sum_i C_{\text{old}}(i)G(x; i, \sigma_i)$$  \hspace{1cm} (4–5)

In order to simulate a real detector with Equation 4–5, I needed full-width half-max values for that detector. Table 4-2 shows estimated full-width half-max values for photopeaks in several experimental spectra: Cs-137, Co-60, and Ba-133. FWHM values for other energies can be estimated by linear interpolation between values in Table 4-2.

<table>
<thead>
<tr>
<th>Energy (keV)</th>
<th>Width (keV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>50.0</td>
<td>7</td>
</tr>
<tr>
<td>81.0</td>
<td>9</td>
</tr>
<tr>
<td>302.9</td>
<td>28</td>
</tr>
<tr>
<td>356.0</td>
<td>32</td>
</tr>
<tr>
<td>448.0</td>
<td>42</td>
</tr>
<tr>
<td>661.7</td>
<td>45</td>
</tr>
<tr>
<td>1173.2</td>
<td>68</td>
</tr>
<tr>
<td>1332.5</td>
<td>70</td>
</tr>
</tbody>
</table>

The Gaussian transformation described in Equation 4–5 works very well at energies greater than around 200 keV. At lower energies, however, photopeaks are noticeably skewed in the low-energy direction. A more complicated transformation, described in Equation 4–6 and illustrated in Figure 4-6, compensates for such low-energy tailing with two additional parameters, $R_{\text{tail}}$ and $\sigma_{\text{tail}}$ ($= \text{FWHM}_{\text{tail}}/2.35$), which control the prominence and length of the low-energy tail.
\[ C_{new}(x) = \sum_i C_{old}(i) \begin{cases} \ G(x; i, \sigma_i)(1 - R_{tail}) + G(x; i, \sigma_{tail})R_{tail}, & \text{if } x < i \\ G(x; i, \sigma_i), & \text{otherwise} \end{cases} \]  

(4-6)

Figure 4-6. The right side is a Gaussian with standard deviation \( \sigma \), and the left side is the sum of two Gaussians with standard deviations \( \sigma \) and \( \sigma_{tail} \). The tailing ratio \( R_{tail} \) in this case is 0.25, meaning that the Gaussian with standard deviation \( \sigma_{tail} \) makes up one-quarter of the total height at the center.

For our detector, \( R_{tail} \) is 0.25 and \( FWHM_{tail} \) is 23 keV. After applying a transformation for electronic broadening, the detector response functions can be used individually or combined to simulate complete detector spectra for any incident gamma-ray spectrum.
4.5 Complete Detector Spectra

The detector response functions described in Section 4.4 can be combined to simulate complete detector spectra for any gamma source. Such spectra could be compared with experimental detector spectra to validate our detector response function generation capability. We could also simulate spectra for isotopes that are not available in our lab, creating a library of test cases for our peak search capability (discussed in a later chapter). Figure 4-7 shows a simulated detector spectrum for Ba-133. For comparison, Figure 4-8 shows an real detector spectrum obtained with a 5cmx5cm square cylindrical NaI detector.

![Simulated detector response for Ba-133](image)

**Figure 4-7.** Simulated detector response for Ba-133, combining detector response functions for eight emission energies.

There are two significant differences between the simulated detector response in Figure 4-7 and the measured detector response in Figure 4-8. The measured detector
Figure 4-8. Measured detector response spectrum for Ba-133, for comparison with the simulated detector response in Figure 4-7.

response has a very large peak at 30 keV, while the simulated detector response has a much smaller peak at the same position. The measured detector response also has a small, broad peak at 160 keV.

4.6 Applications for Synthetically Generated Detector Response Functions

Synthetically generated detector response functions play a central role in the Advanced Synthetically Enhanced Detector Resolution Algorithm (ASEDRA). Synthetically generated response functions for monoenergetic sources are used as part of the peak search algorithm, allowing ASEDRA to strip away all of the secondary features associated with each identified photopeak. Synthetically generated response functions for complete nuclides can be used as sample data against which to test the algorithm.
CHAPTER 5
PEAK SEARCH ALGORITHM

The preceding chapters have described foundational capabilities: removing stochastic noise from spectra, simulation of monoenergetic detector response functions, and simulation of complete detector spectra. The advanced synthetically enhanced detector response algorithm (ASEDRA) uses these foundational capabilities for peak search. ASEDRA’s strategy is to break the problem of spectral deconvolution into smaller problems and solve each problem individually, as shown in Figure 5-1. First, the adaptive chi-processed (ACHIP) denoising algorithm, described in Chapter 3, is applied to both measured spectra: the sample spectrum and the background spectrum. Then, the background spectrum is subtracted from the sample spectrum. Finally, the problem of deconvolving photopeaks from the sample is solved by a recursive algorithm that finds and strips away one photopeak at a time.

Background spectra usually have higher counting times than sample spectra, so the number of counts in a background spectrum must be scaled down accordingly before background subtraction. The rescaling and subtraction is performed as described by Equation 5–1. The significance factor should ordinarily be set to 1.0, but may be increased to account for uncertainty in the background spectrum due to environmental changes. The channel index is represented by $i$.

$$
(Sample_{new})_i = (Sample_{old})_i - (Background)_i \cdot (Significance\ Factor) \cdot \frac{Time_{sample}}{Time_{background}}
$$

A copy of the sample spectrum is created to represent the portion of the sample spectrum that has not yet been attributed to incident radiation; that copy is called the remainder.

The ASEDRA algorithm searches for a photopeak, starting at the high energy end of the remainder spectrum. ASEDRA identifies, as a photopeak, the first channel to meet the
Figure 5-1. Advanced synthetically enhanced detector resolution algorithm flow diagram.
following two criteria. First, the remainder has more counts at that channel than at any
other channel within a distance of half of the full-width half-max. Second, the number of
counts in the remainder at that channel is greater than $T_{abs} + S_i \cdot T_{rel}/100$, where $T_{abs}$ is
the absolute threshold, $S_i$ is the counts in the sample spectrum for that channel, and $T_{rel}$
is the relative threshold. Thresholds are described further in Section 5.1.

If no peak is found, then the ASEDRA algorithm terminates. Otherwise, if a peak
is found, its position and height must be characterized. The position is the channel
which met the two criteria described in the previous paragraph. The height of the
photopeak is the number of counts in the remainder at that channel. After the photopeak
is characterized, a detector response function for that peak is generated, as described in
Chapter 4, and subtracted from the remainder spectrum. Then the peak search starts over
with the new remainder.

### 5.1 Input Files

The ASEDRA program uses five input files: settings, sample spectrum, background
spectrum, resolution calibration, and energy calibration. The settings file is always called
“process.txt.” An example of a “process.txt” settings file is shown in Figure 5-2.

The first two settings in “process.txt” are pathnames for the sample and background
spectra. These two files use the Maestro file format to represent count times, counts as a
function of channel, and other information related to measured detector spectra.

The third setting in “process.txt” is the background significance factor, a floating-
point scale factor, which is used in Equation 5–1. The background significance factor
is ordinarily set to 1.0, but can be adjusted to compensate for changes in background
radiation levels. In this case, a setting of 0.0 completely turns off background subtraction.

The fourth setting in “process.txt” is the pathname for the resolution calibration,
which in this case is set to “fwhm.txt.” An example resolution calibration file, in Figure 5-
3, has two columns representing energy and full-width half-max. This file provides
Figure 5-2. Advanced synthetically enhanced detector resolution algorithm settings file, which is always named “process.txt.”

resolution information at various energies, and ASEDRA fills in the gaps by linear interpolation between adjacent points.

The fifth setting in “process.txt” is a pair of tailing parameters, $R_{\text{tail}}$ and $FWHM_{\text{tail}}$, that are described in Section 4.4.

The sixth setting in “process.txt” is the pathname for the energy calibration, which in this case is set to “1k.txt.” An example energy calibration file, in Figure 5-4, has two columns representing channel and energy. This file indicates the energy, in keV, associated with various channels, and ASEDRA fills in the gaps by linear interpolation between adjacent points.

The seventh setting in “process.txt” controls denoising. A positive value becomes the chi-squared threshold described in Sections 3.2 and 3.3 and turns on the CHIP denoising algorithm. A value of 0 completely turns off denoising, and a negative value turns on the ACHIP denoising algorithm, which is described in Section 3.4. If the ACHIP algorithm is
turned on, the eighth setting controls the value of $\alpha$, which is the probability for any given channel that stochastic noise will be treated as a real feature. Smaller values of $\alpha$ allow more denoising, but may also lead to real features being smoothed away. Note that the certainty described in Sections 3.2, 3.3, and 3.4 is equal to $1 - \alpha$.

The ninth setting in “process.txt” indicates the material for a shield placed between the sample and detector. So far, ASEDRA only understands two material types: (0) air
and (1) iron. Additional Monte Carlo N-particle (MCNP) simulations are required in order to support other material types.

The tenth and eleventh settings in “process.txt” are the absolute ($T_{abs}$) and relative ($T_{rel}$) thresholds that were described as part of the peak search algorithm at the beginning of this chapter. ASEDRA ignores any peaks shorter than the absolute threshold or shorter than the total spectrum multiplied by the relative threshold (as a percent).

Sometimes, actual environmental conditions are different than those that were used in the MCNP simulations. The final setting, a scattered count scale factor provides a way to adjust the number of non-photopeak counts in generated detector response functions to account for scattering in the environment. A negative setting tells ASEDRA to perform the adjustment automatically, but this feature is crudely implemented and not yet reliable. The value of 1 just turns off this feature. The scattered counts scale factor is discussed further in Chapter 10 as a possibility for additional research.

### 5.2 Example

The following illustrations shown an approximation of an actual ASEDRA analysis for a synthetically generated Ba-133 spectrum and are meant to demonstrate the details of how the ASEDRA algorithm works. This analysis used the input files presented in Section 5.1, in which both denoising and background subtraction are turned off. Actual ASEDRA results are shown in later chapters.

The original measured spectrum is shown in Figure 5-5 and starts out equal to the remainder spectrum. There are eight local maxima points on the spectrum. Of those local maxima, the highest energy is at 356 keV. The height of the remainder spectrum at that point is 1650 counts, so the first identified peak is characterized as having a photopeak energy of 356 keV and a peak height of 1650 counts.

The detector response function for the first identified photopeak is shown in Figure 5-6. Note that the local maximum near 200 keV in the original measured spectrum is due to the Compton edge of this 356 keV photopeak.
The 356 keV photopeak is subtracted from the remainder spectrum, yielding a new remainder spectrum that is shown in Figure 5-7. The highest-energy local maximum in the remainder is at 384 keV. The remainder has 196 counts at that energy, so a second peak is identified with an energy of 384 keV and a height of 196 counts, as shown in Figure 5-8.

The 384 keV photopeak is subtracted from the remainder spectrum, yielding a new remainder spectrum that is shown in Figure 5-9. The highest-energy local maximum in the remainder is at 301 keV. The remainder has 681 counts at that energy, so a third peak is identified with an energy of 301 keV and a height of 681 counts, as shown in Figure 5-10.

The 301 keV photopeak is subtracted from the remainder spectrum, yielding a new remainder spectrum that is shown in Figure 5-11. The highest-energy local maximum
Figure 5-6. Remainder spectrum is shown in blue and is identical to the original sample spectrum. The first identified peak is shown in red.

in the remainder is at 275 keV. The threshold is 46.6 counts, ten counts plus 10% of the 366 counts at 275 keV in the original measured spectrum. The remainder has 301 counts at 275 keV, which is higher than the threshold value of 46.6 counts, so a fourth peak is identified with an energy of 275 keV and a height of 301 counts, as shown in Figure 5-12.

The 275 keV photopeak is subtracted from the remainder spectrum, yielding a new remainder spectrum that is shown in Figure 5-13. The highest-energy local maximum in the remainder is at 223 keV. The threshold is 14 counts, ten counts plus 10% of the 40 counts at 223 keV in the original measured spectrum. The remainder has ten counts at 223 keV, which is lower than the threshold value of 14 counts, so this local maximum is not identified as a photopeak.
Figure 5-7. Original sample spectrum is shown in blue. The remainder spectrum, after subtracting the first identified peak, is shown in red.

The next highest-energy local maximum in the remainder is at 161 keV. The threshold is 23.6 counts, ten counts plus 10% of the 136 counts at 161 keV in the original measured spectrum. The remainder has ten counts at 161 keV, which is lower than the threshold value of 23.6 counts, so this local maximum is not identified as a photopeak.

The next highest-energy local maximum in the remainder is at 81 keV. The threshold is 538 counts, ten counts plus 10% of the 5280 counts at 81 keV in the original measured spectrum. The remainder has 5100 counts at 81 keV, which is higher than the threshold value of 538 counts, so a fifth peak is identified with an energy of 81 keV and a height of 5100 counts, as shown in Figure 5-14.
Figure 5-8. Remainder spectrum is shown in blue. The second identified peak is shown in red.

The 81 keV photopeak is subtracted from the remainder spectrum, yielding a new remainder spectrum that is shown in Figure 5-15. The highest-energy local maxima in the remainder are at 161 keV and 223 keV, at which the remainder heights of ten counts and ten counts are lower than the threshold values of 23.6 counts and 14 counts. The next highest-energy local maximum in the remainder is at 53 keV. The threshold is 79.9 counts, ten counts plus 10% of the 699 counts at 53 keV in the original measured spectrum. The remainder has 450 counts at 53 keV, which is higher than the threshold value of 79.9 counts, so a sixth peak is identified with an energy of 53 keV and a height of 450 counts, as shown in Figure 5-16.
The 53 keV photopeak is subtracted from the remainder spectrum, yielding a new remainder spectrum that is shown in Figure 5-17. There are two local maxima in the remainder at 161 keV and 223 keV, at which the remainder heights of ten counts and ten counts are lower than the threshold values of 23.6 counts and 14 counts. Therefore, the ASEDRA algorithm can not find any additional photopeaks.

This chapter describes how the ASEDRA algorithm works, bringing together capabilities such as denoising and response function generation for the purpose of spectral deconvolution. The following three chapters show how that algorithm performs on a variety of example spectra.
Figure 5-10. Remainder spectrum is shown in blue. The third identified peak is shown in red.
Figure 5-11. Original sample spectrum is shown in blue. The remainder spectrum, after subtracting the first three identified peaks, is shown in red.
Figure 5-12. Remainder spectrum is shown in blue. The fourth identified peak is shown in red.
Figure 5-13. Original sample spectrum is shown in blue. The remainder spectrum, after subtracting the first four identified peaks, is shown in red.
Figure 5-14. Remainder spectrum is shown in blue. The fifth identified peak is shown in red.
Figure 5-15. Original sample spectrum is shown in blue. The remainder spectrum, after subtracting the first five identified peaks, is shown in red.
Figure 5-16. Remainder spectrum is shown in blue. The sixth identified peak is shown in red.
Figure 5-17. The original sample spectrum is shown in blue. The remainder spectrum, after subtracting all six identified peaks, is shown in red. No additional peaks can be identified because the remaining peaks at 161 keV and 223 keV are below the threshold for peak identification.
CHAPTER 6
PEAK SEARCH WITH SIMULATED SPECTRA AND NO NOISE

A variety of factors can complicate analysis of experimental detector responses: background radiation, stochastic noise, uncertainties in the detector responses for monoenergetic components, variability in scatter or shielding from the surrounding environment, and uncertainty in the sample composition. All of these complicating factors can be removed by testing the advanced synthetically enhanced detector resolution algorithm (ASEDRA) against simulated detector responses, as described in Section 4.5, so that any error is attributable solely to the peak search algorithm. Later chapters will bring such complicating factors back into the picture so that ASEDRA’s overall performance can be judged, and so that it will be clear, for the sake of guiding further research, which complicating factors have the greatest impact on ASEDRA’s performance.

6.1 Cesium-137

Cs-137 provides a very simple example for peak search because it has only one visible photopeak. A Cs-137 detector spectrum can be simulated with the spectral generator described in Section 4.5 and the sample description in Figure 6-1, which indicates that there is a single peak at 661.7 keV with a height of 650 counts.

![Image of generate.txt file](image)

Figure 6-1. Input file for generating a simulated Cs-137 detector response function. The first column lists the energies, in keV, of the photopeaks. The second column lists the photopeak heights in counts.

The process.txt input file, shown in Figure 6-2, provides information about the sample and the detector, indicates where other input files can be found, and allows some tuning
of ASEDRA’s behavior. Each of the input parameters found in process.txt is described in Chapter 5. In this case, the background significance factor is set to 0 so that the background file will be ignored. This setting makes sense for a synthetically simulated spectrum, for which there is no background. In this chapter, the chi-squared threshold is set to 0, which turns off denoising, because the spectra in this section have no stochastic noise.

![Figure 6-2. Input settings file for simulated Cs-137.](image)

Resolution for a particular detector varies as a function of energy. The full-width half-max calibration function, measured in keV and provided as a function of energy (keV), is defined in the file fwhm.txt, as indicated by process.txt. The FWHM calibration file is shown in Figure 6-3.

The spectral deconvolution process for the simulated Cs-137 spectrum in Figure 6-4 has only a few simple steps. First, ASEDRA scans the spectrum, starting at the high energy end, searching for a channel which meets the following conditions: more counts than any other channel within one FWHM, more counts than the rejection threshold, and more counts than the relative channel threshold times the number of counts in the original spectrum at that channel divided by one hundred. The first channel to meet all three of

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample file</td>
<td>&quot;generated-maestro.txt&quot;</td>
</tr>
<tr>
<td>Sample Exposure Time</td>
<td>3</td>
</tr>
<tr>
<td>Background File</td>
<td>&quot;examples/spectra/background/rd-bkg-1k-10m-y-0.Spe&quot;</td>
</tr>
<tr>
<td>Background Exposure Time</td>
<td>0</td>
</tr>
<tr>
<td>Background Significance Factor (1 for correct background subtraction)</td>
<td>0</td>
</tr>
<tr>
<td>Max energy FWHM calibration table: file in &quot;position(keV) width(keV)&quot; format</td>
<td>fwhm.txt</td>
</tr>
<tr>
<td>Low energy tailing: height ratio, NFWH(keV)</td>
<td>0.25</td>
</tr>
<tr>
<td>Energy calibration table</td>
<td>LK.txt</td>
</tr>
<tr>
<td>Chi-squared threshold (-1 switches to adaptive, 0 is no denoising)</td>
<td>0</td>
</tr>
<tr>
<td>Alpha value for Adaptive Chisq (used if chi-threshold set to -1, max smoothing is 0.005, min smoothing is 0.1)</td>
<td>0.005</td>
</tr>
<tr>
<td>Shielding Material (0=air,1=iron)</td>
<td>0</td>
</tr>
<tr>
<td>Rejection threshold (minimum peak height)</td>
<td>10</td>
</tr>
<tr>
<td>Relative Channel Threshold (minimum percent of spectrum at that channel)</td>
<td>10</td>
</tr>
<tr>
<td>Scattered counts scale factor to account for unknown geometry (1 for no effect, -1 switches to adaptive)</td>
<td>1</td>
</tr>
</tbody>
</table>
Figure 6-3. Detector resolution calibration data.

these conditions is at 662 keV, and ASEDRA reports a photopeak at that location with a height equal to the counts per channel at the photopeak’s centroid. Next, ASEDRA creates a matching 662 keV detector response function as in Chapter 4 and subtracts that detector response function from the spectrum. Peak search is repeated on the remainder, but this time no channels match the conditions for finding a photopeak. The peak search is complete.

Spectral deconvolution is very simple for Cs-137 because there is only one photopeak. Next, I demonstrate spectral deconvolution for the slightly more complicated case of Co-60, which has two photopeaks.

6.2 Cobalt-60

Co-60 has two photopeaks at 1173 keV and 1332 keV, as shown in Figure 6-5. After the first peak at 1332 keV is found and subtracted from the spectrum (ASEDRA starts at the high energy end), the peak search continues on the remainder. Next, ASEDRA finds the 1173 keV photopeak and subtracts it as well. Finally, the remainder contains no channels which meet the conditions for identifying a photopeak, and the deconvolution process is complete. The results are shown in Figure 6-6.
Figure 6-4. Advanced synthetically enhanced detector resolution algorithm (ASEDRA) results overlayed on the original simulated Cs-137 detector response function. The simulated response function is shown in red. ASEDRA found only one peak, at 661 keV, which is shown as a red line whose height indicates the height of the identified photopeak.

Figure 6-5. Input file for generating a simulated Co-60 detector response function. The first column lists the energies, in keV, of the photopeaks. The second column lists the photopeak heights in counts.
Figure 6-6. Advanced synthetically enhanced detector resolution algorithm (ASEDRA) results overlayed on the original simulated Co-60 detector response function. ASEDRA found both peaks: 1173 keV and 1332 keV.

6.3 Barium-133

Ba-133 presents a more interesting case study: six photopeaks, some of which are overlapping. The two highest energy peaks are at 356 keV and 384 keV. Note in Figure 6-8 that these two peaks are overlapping. Although the highest energy photopeak is at 384 keV, the photopeak at 356 keV is found first. After the 356 keV peak is found and stripped away, the 384 keV peak is exposed and can be found next.

These case studies show that, given ideal conditions, the ASEDRA algorithm performs very well. Complications are added gradually in the following two chapters, demonstrating how ASEDRA copes with each challenge.
Figure 6-7. Input file for generating a simulated Ba-133 detector response function. The first column lists the energies, in keV, of the photopeaks. The second column lists the photopeak heights in counts.

<table>
<thead>
<tr>
<th>Energy (keV)</th>
<th>Counts</th>
</tr>
</thead>
<tbody>
<tr>
<td>53</td>
<td>450</td>
</tr>
<tr>
<td>81.0</td>
<td>5100</td>
</tr>
<tr>
<td>160.6</td>
<td>10</td>
</tr>
<tr>
<td>223.2</td>
<td>10</td>
</tr>
<tr>
<td>276.4</td>
<td>310</td>
</tr>
<tr>
<td>302.9</td>
<td>660</td>
</tr>
<tr>
<td>356</td>
<td>1620</td>
</tr>
<tr>
<td>383.8</td>
<td>200</td>
</tr>
</tbody>
</table>
Advanced synthetically enhanced detector resolution algorithm (ASEDRA) results overlayed on the original simulated Ba-133 detector response function. ASEDRA found all of the photopeaks, including the overlapping peaks at 276/303 keV and 356/384 keV.
CHAPTER 7
PEAK SEARCH WITH SIMULATED SPECTRA AND NOISE

A advanced synthetically enhanced detector resolution algorithm (ASEDRA) performed very well with simulated spectra in Chapter 6. Next, I explore ASEDRA’s response to noise by adding stochastic noise to the example spectra.

The process.txt file in Figure 7-1 is changed only slightly from the previous chapter. Adaptive chi-processed (ACHIP) denoising is turned on by setting the chi-squared threshold to -1. The alpha(\(\alpha\)) parameter indicates the relative importance of removing noise and preserving real features. Further discussion of \(\alpha\) can be found in Chapter 3.

Figure 7-1. Adaptive denoising is turned on by setting the chi-squared threshold to -1. All other settings are identical to the settings in the previous chapter.

Counts in each channel of the example spectra from the previous chapter are randomly shifted according to a Poisson probability distribution. Ideally, the ACHIP denoising algorithm should completely remove the effects of that noise. The ACHIP algorithm is far from perfect, however, and ASEDRA must cope with the difference.

7.1 Cesium-137

The Cs-137 response function, with Poisson noise added, is shown in Figure 7-2. The results of denoising, followed by spectral deconvolution, are shown in Figure 7-3. ACHIP
denoising removed most of the stochastic noise, and ASEDRA correctly identified the photopeak at 661 keV.

7.2 Cobalt-60

The Co-60 response function, with Poisson noise added, is shown in Figure 7-4. The results of denoising, followed by spectral deconvolution, are shown in Figure 7-5. ACHIP denoising removed most of the stochastic noise, and ASEDRA correctly identified both of the photopeaks.

7.3 Barium-133

ASEDRA performed well with the noisy Cs-137 and Co-60 spectra, but Ba-133 is far more difficult. Figure 7-6 shows the noisy Ba-133 spectrum, and the stochastic noisy
Figure 7-3. Advanced synthetically enhanced detector resolution algorithm (ASEDRA) results overlayed on the denoised version of the simulated Cs-137 detector response function in Figure 7-2. ASEDRA found the only photopeak at 661 keV.

makes the overlapping peaks even less distinguishable. Figure 7-7 shows that the first two photopeaks at 356 keV and 384 keV are correctly identified. The next photopeak to be identified is at 303 keV, but its position is incorrectly characterized as 299 keV, leading to a slightly incorrect subtraction of the 303 keV response function. That difference leaves some counts in the remainder at 316 keV, which are incorrectly identified as a photopeak. The results are similar in Figure 7-8, for which denoising was not used.

ASEDRA makes mistakes when analyzing a one-minute Ba-133 spectrum, so I also show ASEDRA’s performance with the five-minute spectrum in Figure 7-9, which has less stochastic noise.
The ASEDRA results on a five-minute Ba-133 spectrum are similar to the results for a one-minute spectrum, as shown in Figure 7-10. The results for analyzing the same spectrum without denoising are shown in Figure 7-11. Without denoising, the 303 keV photopeak is correctly characterized, and no false photopeak is identified at 316 keV. In this case, denoising actually makes the situation worse. One explanation is that the photopeaks at 276 keV and 303 keV form a shape which is not well modelled by a set of parabolas. Perhaps a denoising tool that uses higher order polynomials would do a better job on this problem.

Several case studies in this Chapter demonstrate ASEDRA’s performance under conditions that are ideal except for synthesized stochastic noise. A variety of other
Figure 7-5. Advanced synthetically enhanced detector resolution algorithm (ASEDRA) results overlayed on the denoised version of the simulated Co-60 detector response function in Figure 7-4. ASEDRA found both photopeaks at 1176 keV and 1336 keV.

Factors can complicate spectral deconvolution: changes in the background radiation, scattered radiation from nearby objects in the lab, and uncertainty in the energy and FWHM calibration curves. The next chapter includes all of these complicating factors by using laboratory measurements with a real NaI scintillation detector. Additionally, a plutonium beryllium source is introduced as an example of a particularly convoluted detector spectrum.
Figure 7-6. Simulated, one-minute, Ba-133 detector response function with Poisson noise.
Figure 7-7. Advanced synthetically enhanced detector resolution algorithm results overlayed on the denoised version of the simulated, one-minute Ba-133 detector response function in Figure 7-6.
Figure 7-8. Advanced synthetically enhanced detector resolution algorithm results for the simulated, one-minute Ba-133 detector response function in Figure 7-6. Denoising was not used for these results.
Figure 7-9. Simulated, five-minute, Ba-133 detector response function with Poisson noise.
Figure 7-10. Advanced synthetically enhanced detector resolution algorithm results overlayed on the denoised version of the simulated Ba-133 detector response function in Figure 7-9.
Figure 7-11. Advanced synthetically enhanced detector resolution algorithm results for the simulated, five-minute Ba-133 detector response function in Figure 7-9. Denoising was not used for these results.
CHAPTER 8
PEAK SEARCH WITH MEASURED DETECTOR SPECTRA

Previous chapters used idealized examples for demonstrating how the advanced synthetically enhanced detector resolution algorithm (ASEDRA) performs spectral deconvolution. A variety of additional complications arise in real laboratory conditions: changes in the background radiation, scattered radiation from nearby objects in the lab, and uncertainty in the energy and full-width half-max (FWHM) calibration curves. This chapter includes laboratory measurements, with a 5 cm square cylindrical NaI detector, of samples which are similar to the examples in previous chapters. Additionally, a plutonium beryllium source is included to show ASEDRA’s performance on a highly convoluted detector spectrum.

Energy calibration becomes more significant when real detectors are used. Table 8-1 shows the energy calibration data for the examples in this chapter.

<table>
<thead>
<tr>
<th>Channel</th>
<th>Energy (keV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>62</td>
<td>53.2</td>
</tr>
<tr>
<td>97</td>
<td>81.0</td>
</tr>
<tr>
<td>334</td>
<td>302.9</td>
</tr>
<tr>
<td>387</td>
<td>356.0</td>
</tr>
<tr>
<td>705</td>
<td>661.7</td>
</tr>
<tr>
<td>1239</td>
<td>1173.2</td>
</tr>
<tr>
<td>1402</td>
<td>1332.5</td>
</tr>
</tbody>
</table>

8.1 Cesium-137

A measured Cs-137 spectrum is shown in Figure 8-1, and the corresponding ASEDRA results are shown in Figure 8-2. ASEDRA finds the 662 keV photopeak, as before, but it also finds an additional features at 292 keV. The additional feature at 292 keV has a height of only 12 counts, only two counts above the threshold for rejection.

8.2 Cobalt-60

A measured Co-60 spectrum is shown in Figure 8-3. Unlike the simulated spectra in the previous chapters, the measured Co-60 spectrum has a broad peak between 200 keV
and 350 keV. The ASEDRA results in Figure 8-4 show three features in this region: 208 keV, 233 keV, and 272 keV. These features may be the result of scattering from objects that were not included in the MCNP simulations. Each of these three features has a height of less than 15 counts.

8.3 Barium-133

A measured Ba-133 spectrum is shown in Figure 8-5, and the corresponding ASEDRA results are shown in Figure 8-6. ASEDRA incorrectly characterizes the 303 keV photopeak as having a position of 299 keV, as in the previous chapter, and, consequently, identifies an additional false photopeak at 316 keV. ASEDRA also identifies six very small features between 100 keV and 250 keV. The source of these additional features is not known.
Figure 8-2. Advanced synthetically enhanced detector resolution algorithm (ASEDRA) results overlayed on the denoised version of the measured, one-minute Cs-137 detector response function in Figure 8-1. ASEDRA found the only photopeak at 661 keV. The additional peak at 290 keV is only two counts above the rejection threshold and is not real.

8.4 Plutonium Berillium (PuBe)

Detector spectra in previous sections and chapters came from well known sources to facilitate evaluation of ASEDRA’s performance. An additional detector spectrum, using a plutonium berillium source, is shown in Figure 8-7, and the corresponding ASEDRA results are shown in Figure 8-8. The exact composition of the Plutonium Berillium (PuBe) source and its radiation spectrum are topics of current investigation, so ASEDRA’s results are compared with a high-purity Germanium spectrum for the same sample in Figure 8-9.
Figure 8-3. Measured, one-minute, Co-60 detector response function.

Without proper energy calibration for the Germanium detector, it is difficult to determine how closely the ASEDRA results match the Germanium results. However, while some skepticism is warranted, the similarities shown in Figure 8-9 are very encouraging.

I tried simulating a plutonium beryllium spectrum that includes only the labelled photopeaks in Figure 8-9, which match photopeaks in the HPGe detector spectrum. The simulated plutonium beryllium spectrum and associated ASEDRA results are shown in Figure 8-10, from which two very interesting conclusions can be drawn.

First, the simulated plutonium beryllium spectrum in Figure 8-10 has noticeable gaps compared to the measured spectrum in Figures 8-8 and 8-9. This shows that there are additional photopeaks, not visible in the HPGe spectrum, which have a significant effect
Figure 8-4. Advanced synthetically enhanced detector resolution algorithm (ASEDRA) results overlayed on the denoised version of the measured, one-minute Co-60 detector response function in Figure 8-3. ASEDRA found both primary photopeaks at 1176 keV and 1336 keV. The additional three photopeaks between 200 keV and 300 keV are unidentified, but this spectrum clearly contains more features than can be explained by Co-60 alone.

on the NaI spectrum. At least some of the extra peaks in Figure 8-10, which do not match HPGe peaks, must be real photopeaks that were identified by ASEDRA. This means that ASEDRA can deconvolve photopeaks from a low-resolution NaI detector that are not visible on a high-resolution HPGe detector.

Second, ASEDRA results show very high reliability. In a highly convoluted detector spectrum with twenty-two photopeaks, ASEDRA correctly identified all but three photopeaks with no false positives.
This chapter demonstrated ASEDRA’s capabilities on real laboratory data, collected with a NaI scintillation detector, as well as on a highly convoluted simulation spectrum. There remains room for improvement, but these results demonstrate a significant capability for energy resolution enhancement. In particular, ASEDRA is designed to work reliably within time and cost constraints: rapid execution, tolerance of short counting times, and resolution enhancement for relatively inexpensive detectors.
Figure 8-6. Advanced synthetically enhanced detector resolution algorithm (ASEDRA) results overlayed on the denoised version of the measured, one-minute Ba-133 detector response function in Figure 8-5. ASEDRA correctly extracted the overlapping photopeaks at 356 keV and 384 keV. ASEDRA incorrectly indicated that the 303 keV photopeak was at 298 keV. Incorrect subtraction of the 303 keV photopeak led to a false positive at 316 keV, but the 276 keV photopeak was still correctly identified.
Figure 8-7. Measured, one-minute, PuBe detector response function.
Figure 8-8. Advanced synthetically enhanced detector resolution algorithm results overlayed on the denoised version of the measured, one-minute PuBe detector response function in Figure 8-7.
Figure 8-9. Advanced synthetically enhanced detector resolution algorithm results from Figure 8-8 compared with a denoised, higher resolution (Germanium), but uncalibrated spectrum for the same sample. Labels are provided to indicate peaks that appear to match between the two spectra.
Figure 8-10. Advanced synthetically enhanced detector resolution algorithm (ASEDRA) results for a simulated PuBe spectrum with no stochastic noise. ASEDRA made only three mistakes. A small photopeak around 150 keV that should have been between Q and S was misplaced. Two other small photopeaks, G and I, were not identified. Labels in this figure match the labels in Figure 8-9.
The advanced synthetically enhanced detector resolution algorithm (ASEDRA) consists of a spectral deconvolution algorithm, as well as other foundational capabilities upon which the deconvolution algorithm is built. Although these foundational capabilities were developed in support of spectral deconvolution research, they are also useful as independent tools.

9.1 Adaptive Chi-Processed (ACHIP) Denoising

ASEDRA needed a denoising component because early versions of the deconvolution algorithm were highly sensitive to stochastic noise. Despite improvements in the deconvolution algorithm, denoising remains useful for delivering results on very low count spectra. The ACHIP denoising algorithm is also useful as a standalone tool for rapid processing of one-dimensional data with a Poisson noise component. Additional research will soon allow analysis of higher dimensional data, and possibly analysis of data with non-Poisson noise.

9.2 Detector Response Generation

The accurate generation of monoenergetic response functions has been extremely useful for spectral deconvolution. ASEDRA’s spectral deconvolution algorithm starts at the high energy end of a detector spectrum, so that it finds photopeaks before other components of the detector response function, such as Compton edges. As each photopeak is found, ASEDRA strips away the entire detector response function associated with each photopeak, so that a Compton edge is never found and mistakenly identified as a photopeak. In addition to its usefulness within ASEDRA, detector response generation is useful for detector calibration or for providing synthetic test cases for spectral analysis.

Detector response function generation provides a very precise method for calibrating detectors. A synthetically generated spectrum, based on an estimate of the calibration functions (both energy and resolution), can be overlayed on a measured calibration spectrum for comparison. Even slight differences between the two spectra are easily visible.
and suggest improvements to the calibration functions. This process is repeated until a close match between synthetic and measured spectra indicates that calibration is finished.

Generating synthetic detector spectra is much faster and easier than measuring spectra in the lab. Additionally, the results are more controllable and repeatable. Such synthetic spectra provide useful test cases for a deconvolution algorithm.

9.3 Detector Spectrum Deconvolution

ASEDRA’s deconvolution algorithm is a simple method for taking advantage of the core tools upon which it is built: ACHIP denoising and synthetic generation of detector response functions. Despite its simplicity, ASEDRA has a demonstrated capability for deconvolving intricate detector spectra.

Unfortunately, ASEDRA is also very sensitive to mistakes in resolution calibration. A low estimate of the full-width half-max causes single photopeaks to be interpreted as double or (more commonly) triple photopeaks. A high estimate of the full-width half-max prevents ASEDRA from deconvolving overlapping photopeaks. This sensitivity to resolution calibration is important because a detector’s resolution can change from one day to the next and because detector operators are accustomed to thinking of resolution as merely an indication of equipment quality, rather than as an experimental parameter that needs to be precisely characterized.

Adapting to changes in detector resolution is a difficult problem that will require further research. Fortunately, ASEDRA’s simple and highly modular design is very conducive to experimentation with new ideas.
CHAPTER 10
FUTURE WORK

The advanced synthetically enhanced detector resolution algorithm (ASEDRA) has already produced some interesting results, but there is still a great deal of room for improvement. ASEDRA consists of several separate modules, any of which could be separately improved in terms of speed, accuracy, or flexibility. There is also room for experimentation in alternative deconvolution strategies.

10.1 Adaptive Chi-Processed (ACHIP) Denoising

Parabolic fitting is a significant improvement over linear fitting, which in turn was a significant improvement over constant fitting. It is possible that additional increases in polynomial order could lead to further improvement in denoising for detector spectra. Higher order polynomials would allow fitting over a larger number of points, especially in regions of the spectrum with significant curvature. Further research is necessary to determine the ideal polynomial order for this application.

ACHIP denoising relies on chi-squared analysis which, in turn, assumes that each category (channel in this case) has a large number of counts. Spectra with very few counts, or in which low count regions are considered important, may require more rigorous mathematical treatment [15, 16].

Additionally, ACHIP’s denoising strategy could be applied to a wider variety of problems if the algorithm were generalized to support 2D and 3D data.

10.2 Detector Response Generation

Currently, detector response functions are selected according to only photopeak energy and container material. The library could be expanded to include additional materials, and the selection criteria could be further expanded to include other environmental features, such as detector shielding and walls.

ASEDRA would benefit from thorough testing, which could be automatically performed with each code change to determine whether ASEDRA is changing for the better.
ASEDRA’s capability for generating complete detector spectra could be used to develop a suite of synthetic test spectra for more extensive testing.

10.3 Detector Spectrum Deconvolution

Human analysts are intuitively capable of identifying isotopes and deconvolving detector spectra, but such purely intuitive approaches are not amenable to distilling a human analyst’s accumulated wisdom into a fast and precise computer algorithm. Therefore, programmers who tackle the problem of spectral deconvolution generally ignore the expertise of human analysts, turning instead to mathematical techniques such as curve-fitting, fourier analysis, and wavelet analysis.

Perhaps, instead, spectral analysis experts and computer programmers could meet each other half way. Computer programmers could provide tools that are responsible for performing only small pieces of a complete spectral analysis. Spectral analysts could make an effort to use those tools, suggest improvements to the tools, and identify additional parts of the spectral analysis process that could be automated. Such an approach allows spectral analysis tools to evolve in usefulness.

I propose that the foundational tools in the ASEDRA algorithm, such as denoising, background subtraction, detector response function generation, and and subtraction of detector response functions, could be refined for ease-of-use to provide an initial set of tools which human analysts could use and critique. A graphical computer application could provide a human analyst with capabilities for detector response function generation, energy and resolution calibration, and detector response function subtraction. The analyst could make guesses regarding the correct deconvolution, see an overlay of the measured spectrum on a convolution of their guess, and modify each guess to be a closer fit than the previous guess. This process could lead to additional insight into the problem of spectral deconvolution. The experience of analysts could then be distilled into rules for automating the deconvolution process.
A graphical user interface makes the advanced synthetically enhanced detector resolution algorithm (ASEDRA) significantly more accessible. File selection browsers, for example, are a welcome replacement for typing out a file’s full pathname, and radio buttons are more easily understood than a numerical identifier for indicating the type of container. Additionally, it is convenient to change a parameter and see updated results with one push of the “Run ASEDRA” button.

Users must specify four files when using ASEDRA: sample spectrum, background spectrum, energy calibration data, and FWHM calibration data. The graphical interface allows those files to be specified with standard file selection browsers.

ASEDRA needs to know about the sample’s container, in order to select the corresponding set of detector response functions. In process.txt, this selection required typing a number (0=none, 1=iron). Selecting the correct radio button in ASEDRA’s graphical interface is far simpler than remembering such codes. Additional radio buttons will be added as ASEDRA’s library of detector response functions is expanded.

In process.txt, special values are used to turn features on and off. ACHIP denoising is turned on by setting the chi-squared threshold to -1, and turned off by setting the chi-squared threshold to 0. Accidentally using a positive value for the chi-squared threshold activates the obsolete CHIP denoising algorithm. Similarly, tailing correction in process.txt is turned off by setting the tailing height ratio to 0. Both of these controls are much simpler as checkboxes (checked=on, unchecked=off).
Figure A-1. A graphic user interface for ASEDRA is available as an alternative to editing the process.txt file.
REFERENCES


BIOGRAPHICAL SKETCH

Eric Lavigne earned a B.S. in mathematics with a minor in physics from the University of Florida in May 2003. Later, Eric returned to the University of Florida to earn an M.S. in nuclear engineering sciences while studying computer programming on the side. Eric Lavigne and Nong Owens married on Valentine’s Day in 2007. Upon completion of his M.S. program, Eric will work as a programmer for the University of Florida’s Bureau of Economic and Business Research.