R4-B.2: Multi-energy, Limited View Computed Tomography (CT)

I. PARTICIPANTS

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<th>Faculty/Staff</th>
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<tbody>
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<tr>
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<th>Graduate, Undergraduate and REU Students</th>
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II. PROJECT DESCRIPTION

A. Project Overview

The development of energy selective photon counting detectors for X-ray sensing applications has created the possibility for significantly enhancing materials characterization capabilities relative to existing energy integrating or dual-energy systems. Energy integrating methods provide information only regarding material density, while dual energy systems, at best, can image both density and effective atomic number (or equivalently spatial maps of Compton and photoelectric coefficients). In practice, the overlapping nature of the spectra employed in fielded dual energy systems as well as the nature of X-ray physics, significantly complicates the stable recovery of atomic number. As we argue in this report, multi- or hyper-spectral forms of sensing, where data are collected over a large number of narrow energy bins in such a manner as to reflect both attenuation as well as X-ray scattering, have the potential to move X-ray based screening significantly beyond the limitations of the current state-of-the-art systems.

In a bit more detail, the energy integrating and dual-energy methods recover information concerning the object of interest based on the manner in which X-rays are attenuated as they pass through the medium. The attenuation properties in turn reflect both the absorption of the X-rays as well as the scattering of the X-ray photons from the beam. For all fielded X-ray systems in use by DHS, these scattered photons are ignored. It is our hypothesis that there is significant information embedded in these photons; such that their collection and processing can enhance the ability of DHS to characterize materials from X-ray data specifically in the context of limited view systems currently under investigation and development. Indeed, in recent years, DHS has been exploring X-ray systems comprised of spatially fixed sources and detectors in contrast to traditional computed tomography (CT) types of systems where source/detector arrays rotate around the items being scanned. Complicating the development of these systems, the limited number of source-detector paths compared to the full-scale CT case creates substantial challenges in terms of image formation and, ultimately, target detection. As we demonstrate in this report, using the detectors in these systems to collect scattered photons

1The one exception here is the Morpho Yslon XES 3000 system, which collects and processes diffracted photons. As we discuss shortly, the effort in this project is focused not on diffraction, but rather on Compton scattering. While both processes result in photons exiting the main X-ray beam, the physical processes underlying these modalities are distinct. Our focus here is on Compton scattering. Over the long term, there may well be reason to consider fusing data from both of these processes.
photons (in addition to the traditional attenuation-based data) significantly increases the number of "looks" we have at the scene even in these fixed geometries, potentially allowing us to greatly enhance the information content provided by these systems.

In this regard, the most interesting scattering process for the energy range of interest in this application domain, Compton scattering, is characterized by two key properties. First, the intensity of Compton scattering is directly proportional to the electron density in the vicinity of the event. Second, Compton scattering is inelastic, meaning that the energy of the photons shifts after a scattering event, thereby necessitating the use of energy resolving detectors to usefully capture and quantify these processes. The shift in energy determines the direction in which photons are scattered. To a point that we will make more precise shortly, this energy-dependent scattering direction very much "encodes" electron density at a specific location. These two properties have significant systems-level implications for DHS.

Realizing this potential, however, requires that we address a number of challenges. First, the physical processes and mathematical/computational models associated with these scattering processes are more complex than traditional attenuation imaging. The development of a model, which links the observed data to the material properties of interest, is necessary to address the second challenge: how we use these scattered photons in addition to traditional attenuation data to form images. Only after these image formation methods are in place can we quantify the true benefits of these new data; e.g., attainable image resolution and reduction in imaging artifacts, as well as target detection and false alarm rates.

The significance of this project, relative to the larger ALERT program, lies in the potential of these models and associated processing methods to improve the accuracy of screening both checked baggage as well as luggage inspected at the checkpoint. The algorithms at the heart of the current collection of TSA certified systems are not sufficient for the processing of the data that will be produced by the next generation of X-ray scanning systems. Even the state-of-the-art model based iterative reconstruction methods are not designed to fully exploit the information provided by multi-/hyper-spectral X-ray data. Neither are they capable of addressing the challenges encountered when considering the severely limited view of the data provided by these fixed source/fixed detector systems. Our proposed approach to explore the utility of scattered X-ray information to materials characterization is intended to address both of these challenges, and to the best of our knowledge, is the only effort within the ALERT program with this focus.

Finally, we note the steps taken by this team in the area of technology transition. In addition to regular attendance and presentation of this work at the Advanced Development for Security Applications (ADSA) workshops held over the past seven years, Professors Miller and Tracey are partnering with American Science and Engineering (AS&E) and Lawrence Livermore National Laboratory (LLNL) on a soon-to-be awarded project under the 13-05 DHS RFP devoted to the development of next generation X-ray scanning systems. As part of this collaboration, AS&E has committed to collecting data on the system they will be developing, and that will be employed specifically to validate the models and processing methods being developed as part of this project.

While the prototype system being developed under 13-05 funding is mainly focused on Compton scatter tomography as described above, it will also include more traditional transmission measurements. To support processing of transmission data, a Master’s student at Tufts University, Mr. Yaoshen Yuan, recently completed a thesis on the use of energy-discriminating X-ray detectors for improved sinogram decomposition of attenuation data. Although not funded by ALERT, this research is clearly focused on the DHS mission, and we anticipate testing the processing ideas developed in this thesis as part of 13-05. We briefly describe this work in a separate section below.
Biennial Review Results and Related Actions to Address

Strengths

- Modeling of Compton scatter is a complex and challenging task; an accurate and efficient computational model would be quite valuable.
- The investigators have completed literature review and tool development in the first two years of the project, and laid out plans and milestones (development and validation of image formation algorithms) for the coming years. This reviewer agrees with both of them.
- The research methodology has been designed and executed with rigor. The investigators’ technical methodology is sound.
- Researchers presented comprehensive understanding of the field. They have strong background in one of the two main tasks they plan in the coming years: image reconstruction algorithm development. Thus, it is my opinion that they are in a good position to execute the plan.
- Transition pathway partners were clearly identified and use of research results were clearly presented.

Weaknesses and Mitigation

- Weakness: The approach revealed thus far, indicates a highly exploratory methodology and there is some risk that the current path may lead to a negative result.
  - Mitigation: Our work over the past six months has indicated that, in simulation, we can in fact get quite stable and accurate reconstructions of density and photoelectric coefficients from limited angle Compton data especially as supplemented by, again limited view, absorption data. Moreover, in the coming year, our 13-05 collaboration will provide us with real data that will be of use in obtaining a more realistic assessment of the potential of this method. Thus the potential negative results are less and less of a concern.
- Weakness: This project proposes another implementation of limited view CT and hence this reviewer is concerned about replicating other efforts in this area.
  - Mitigation: We are well aware of the state of limited view CT for security scanning at least to the extent to which it has been reported in the open literature. We feel that the approach we offer in its fusion of attenuation data and Compton scattered photons is rather unique.
- Weakness: Transition is implied in the connections made with Analogic and Rapiscan. Although there appears to be active and engaged users, there is no evidence of an understandable agreement between these parties, or a realistic vision/plan for how results will be transitioned.
  - Mitigation: Transition is being affected through the current execution of the joint 13-05 project led by American Science and Engineering (AS&E) with Tufts University as a subcontract. Essentially, AS&E is constructing a scanner that will collect the type of data required by the processing methods being pursued in this ALERT project. The models and processing methods developed with ALERT support are being transferred directly from the graduate student funded by ALERT to the post-doctoral researcher supported by 13-05. To the extent that 13-05 is successful, the methods supported by ALERT will have been transitioned.

State of the Art and Technical Approach

X-ray CT has been used widely in fields ranging from medical imaging [1] and non-destructive evaluation [2] to the investigation of the internal structures of geos-materials [3] and luggage screening [4]; the application of specific interest here. Motivated by a desire to construct spatial maps of materials properties, in recent
years, increased attention has been given to X-ray based approaches in which information is extracted from observations of photons other than those associated with the incident beams. Of particular relevance to this project are X-ray fluorescence computed tomography (XFCT) [5] and Compton scatter tomography [6], each of which is based on distinct physical processes associated with the interaction of X-rays with matter. In the case of XFCT, used for example in micro-tomography applied to analyze biological samples [7], the sample is irradiated with a monochromatic synchrotron beam of low energy (less than 25 keV), which is still greater than the K-shell energy of the elements in the sample. As a result of photoelectric interactions occurring between the X-ray photons and the atoms of the elements, fluorescence X-rays are produced and used as the basis for image reconstruction [8]. For Compton tomography, incoherent scattering [6] is the fundamental physical process giving rise to photons leaving the main beam. This modality has been considered for problems including analyzing human tissues [9]. While Compton scattering is most germane to the ideas we are pursuing for DHS, the mathematics of the models relating observations to material properties for XFCT and Compton tomography are quite similar. Thus, both modalities are informative to our longer term interests in data processing and are reviewed here.

In terms of image reconstruction, a wide range of methods have been considered for both XFCT as well as Compton tomography. In the case of X-ray fluorescence, several different techniques have been developed to recover maps of both attenuation and material density. For example, a statistical approach has been introduced in [10] assuming a Poisson distribution for the data. However, for problems where the K-shell binding energy of the element of interest lays between the emission energy and the K-shell binding energies of the other materials in the sample, it is necessary to update the system matrix at each iteration, which is a time consuming process. Alternatively, an iterative data refinement technique has been provided in [11], which updates the unknown density and fluorescence attenuation at each iteration by minimizing a least square error type of objective function. At each iteration, one of the unknown quantities is replaced with the current value and the equations are solved for the other one. A joint penalized-likelihood Poisson objective function of the unknown element of interest’s density and fluorescence attenuation map is introduced in [12] as a continuation of the work done in [10]. One of the drawbacks of this method is the need to choose a number of parameters, included in the likelihood objective function, to avoid convergence into local minima of the cost function.

In most applications of XFCT, the unknown fluorescence attenuation map has been approximated as a linear combination of the density of the element and a modified version of the absorption attenuation, which may be a good approximation for low energies appropriate for XFCT. It is not at all clear, however, that this approximation is suitable for the higher energies of interest here. Moreover, these studies have been restricted to cases in which a single, monochromatic source is used to illuminate the object which is rotated as a means of acquiring a diversity of views. For DHS applications, more restrictive, limited view geometries are more the norm, and data may be acquired over a range of energies. Thus, while the physical model structure of XFCT and the general iterative reconstruction approaches considered to date are of interest, and will motivate the ideas we consider, significant work remains in terms of adapting and extending these ideas to our application domain.

In addition to XFCT, Compton tomography provides a powerful tool for materials characterization [13]. Most of the research done on Compton scattering tomography can be divided into analytical and numerical approaches. A comprehensive review of the analytical solutions is provided in [14]. The ideas introduced in [15] are the basis of most of the research in the analytical domain. It is shown in [15] that the scattered beams collected by detectors located on a circular arc connecting the source to the detector, called the “isogonic line,” allow for a closed form reconstruction algorithm not unlike conventional filtered backprojection. In a related study, a Radon-transform-like model for a rotating single source/single detector system is introduced in [16] and provides a closed form solution for recovering the electron density on the arcs passing through the source and detector for each point inside the object. Further developments in [17] show that a Chebyshev integral transform is also applicable to the arcs passing through each point inside the object, which confirms
the results provided by [16]. The same idea has been employed in [18] for luggage screening applications. There it was shown that a combination of the proposed method and conventional attenuation tomography can produce a map of atomic numbers. However, the approach is not robust to the noise, necessitating the use of an ad-hoc pre-processing step of smoothing of the data. Although the analytical methods provide efficient, closed form solutions, they can only be applied to very specific data acquisition geometries. Only numerical methods provide the flexibility to robustly process data for the more general class of systems currently of interest to DHS.

In terms of the numerical methods for Compton scatter tomography, most of the work has focused on recovering either the electron density or the total attenuation. A generalized Compton scattering transform that falls in the first category was proposed in [19] to reconstruct the attenuation map of the object of interest. The energy dependency of the attenuation coefficient at the scattering point was not considered there. In [20], the energy dependency of the attenuation is taken into account by approximating the attenuation as a linear function of energy. The algorithm tries to recover the total attenuation coefficient with an iterative minimization method, and performed robustly in the presence of noise. The linear approximation to the attenuation holds in the cases where the range of energy change is small, which again is not the regime of interest in our work. One of the few studies seeking to recover the electron density, combines three different interactions—fluorescence, Compton and absorption—of the X-ray with the elements within the sample [21] to directly estimate the unknown fluorescence attenuation map using Compton scattering measurements. Another approach in X-ray Compton tomography assumes the attenuation coefficient is known from a prior, traditional CT scan, resulting in a linear mapping from density to observations [22]. In addition to ignoring the dependence of attenuation on density, for the limited view problems of interest to us, it is far from clear that a high fidelity attenuation map will be in our possession.

To summarize, the majority of the research to date in the area of Compton tomography focuses on either analytical solutions which are suitable for limited system geometries, or on the recovery of either attenuation or electron density over a limited energy range. We contend that to characterize the materials inside the object of interest for DHS applications, recovery of the electron density (or in our case, the mass density) along with attenuation is essential. Reconstruction of both of these variables has inspired us to develop a Compton scattering tomography model considering both density and photoelectric attenuation coefficients. One of the advantages of including scattering ray paths in the physical model is to increase the success rate of density and attenuation coefficient reconstruction in limited-view and multi-energy data acquisition systems.

![Figure 1: Setup of the sources and detectors. A ray from source $S_1$ to primary detector $D_2$ is scattered with angle $\theta_3$ at the interaction point $r$ and is absorbed by detector $D'$.](image)

We have designed such a limited-view system shown in Figure 1 in which pencil beams produced by each source with a specific energy spectrum, called “primary” raypaths, are scattered in different directions with different energies while passing through the object. We note that the attenuation data collected along these primary raypaths constitute a typical data set for absorption-based X-ray imaging methods. While we will ultimately be interested in using both scatter and absorption data as the basis for estimating density and photoelectric coefficient, here we focus on issues associated with scatter-based imaging. As discussed in our Year 2 project report, the model we have developed which links the number of scattered photons absorbed...
by detector $D'$ to the material properties of interest takes the form:

\[ g(D'_0, E') = \int l_0(E_S) \left[ \int h(D'_0, r, x) S(r, D') h(D, E_S) l_{D_0, D}(r) \rho(r) dr \right] dE_S \tag{1} \]

where

- $l_0(E_S)$ is the initial intensity of the X-ray beam at energy $E_S$;
- $h(D'_0, r, E_S)$ is the attenuation of the beam intensity at energy $E_S$ along the line connecting $r_1$ and $r_2$;
- $\rho(r)$ is the mass density at the interaction point;
- $S(r, \theta, E_S)$ is the scattering factor; and
- $l_{D_0, D}(r)$ is a delta function along the line connecting the source to the primary detector.

The attenuation of the beam intensity $h(D'_0, r_1, E_S)$ along the line connecting $r_1$ and $r_2$ is a function of absorption coefficient $\mu(r, E_S)$ and takes the form:

\[ h(D'_0, r_1, E_S) = \exp \left( -\int \mu(r, E_S) l_{D_0, D}(r') dr' \right) \tag{2} \]

The absorption coefficient itself is the linear combination of Compton and photo-electric absorption as follows:

\[ \mu(r, E_S) = N_A \frac{Z(r)}{M(r)} \mu_{\alpha}(E_S) + \rho(r) \mu_{\beta}(E_S) \tag{3} \]

where $\rho(r)$ is the mass density; $N_A$ is the Avogadro number; $Z(r)$ and $A(r)$ are the atomic number and atomic weight; $\rho(r)$ is the photoelectric coefficients; and $\mu_{\alpha}(E_S) = E_S^{-3}$ and $\mu_{\beta}(E_S)$ is the Klein-Nishina cross section.

The discrete form of the physical model is obtained by discretizing the area to be imaged into a grid of pixels and replacing all integrals by Riemann sum over $E_S$:

\[ g(j, k, E) = \sum_{m} l_0(E_{\text{in}}) \Delta E_S \left[ \sum_{i} h(D'_0, x_i, r_j, k, E_S) S(r_j, \theta_{j, k}, E_S) h(r_j, D, E_S) \delta_{j, k} \rho(r_j) \right] \tag{4} \]

where $\Delta E_S$ is used to discretize $E_S$. Please see our previous report for a full derivation of the model.

Using standard linear algebra, it can be shown that (4) can be formulated as a set of equations nonlinear in the photoelectric coefficient and quasi-linear in density, resulting in a measurement model taking the form:

\[ g = K(\rho, p) \rho + N(0, \delta^2) \tag{5} \]

where $\rho$ and $p$ are lexicographically ordered vectors of density and photoelectric images respectively, and $K(\rho, p)$ is the discretized scattering system matrix obtained from the term $h(D'_0, x, r_j, k, E_S) S(r_j, \theta_{j, k}, E_S) h(r_j, D, E_S)$ in (4).

The vector $g$ is comprised of all of the observed scattered data as a function of source location, secondary detector location, and energy. The total number of elements in $g$ is the number of all possible broken raypaths which is equal to $N_{\text{ray}} = N_x \times N_y \times (N_D - 1)$. More specifically, for the system of interest to us, there will be $N_x \times N_y$ primary raypaths providing absorption-type data. For each of these raypaths, we will collect scattered photons for the remaining $N_D - 1$ detectors. Finally, the measurement noise is modeled as Gaussian distribution with zero mean and $\delta^2$ variance.

In order to recover density and photoelectric images, we solve the following least-squares optimization problem:

\[ (\hat{\rho}, \hat{p}) = \arg\min_{\rho, p} \| g - K(\rho, p) \rho \|_2^2 + R_\rho(\rho) + R_p(p) \tag{6} \]

where $\| g - K(\rho, p) \rho \|_2^2$ measures the mismatch between the data and our prediction of the data for a given $\rho$ and $p$; and $R_\rho(\rho)$ and $R_p(p)$ are regularization terms for density and photoelectric respectively to stabilize the calculation by imposing prior information such as smoothness to the unknown variables $\rho$ and $p$. We have
developed a two-step method for solving this optimization problem. In the first part, density reconstruction is performed. Subsequently, we use this estimate of density to recover the photoelectric coefficient.

### C.1. Density Reconstruction

Our approach to solving (6) is motivated from the physical fact that the impact of the photoelectric coefficient in the data is quite small relative to that of the density especially at higher energy levels. Thus we begin initially by assuming \( p = 0 \), and seek the solution to the following optimization problem:

\[
\hat{p} = \arg\min_{\rho} \| g - K(\rho, 0) \rho \|_2^2 + R_p(\rho). \tag{7}
\]

As it stands, (7) is quasi-linear in the density \( \rho \), in that the density appears nonlinearly in the structure of the matrix \( K \), but also in a linear manner as the vector upon which \( K \) operates. This suggests an iterative approach to solving (7):

1. Assume an initial estimate for the density \( \rho_0 \).
2. Build the matrix \( K(\rho_0, 0) \), which, assuming a quadratic regularizer for density transforms (7) into a linear least squares problem for \( \rho \).
3. Solve the linear least squares problem for the density. In our case we use the LSQR [23] iterative solver owing to the large, sparse nature of the system matrix.
4. If the density has changes, “significantly” update the matrix \( K \) using our new estimate of \( \rho \), and go to step 3, or else exit.

The pseudo code for the iterative approach for solving (7) is given in Table 1.

<table>
<thead>
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<th>Table 1: Pseudo code for iterative quasi-linear solver</th>
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<td><strong>Inputs:</strong></td>
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<td>- ( \rho_0 ) initial estimate of density</td>
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<tr>
<td>- ( \epsilon_0 ) stopping criteria</td>
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<tr>
<td>- ( \epsilon_1 = 1 )</td>
</tr>
<tr>
<td>- ( \epsilon &gt; \epsilon_0 )</td>
</tr>
<tr>
<td><strong>1:</strong> While ( \epsilon &gt; \epsilon_0 )</td>
</tr>
<tr>
<td><strong>2:</strong> Build ( K(\rho_{\epsilon_1-1}, 0) )</td>
</tr>
<tr>
<td><strong>3:</strong> Build ( R_p(\rho_{\epsilon_1-1}) )</td>
</tr>
<tr>
<td><strong>4:</strong> Find ( \rho_{\epsilon_1} ) by solving (7) with LSQR</td>
</tr>
<tr>
<td><strong>5:</strong> Define ( \epsilon := | \rho_{\epsilon_1} - \rho_{\epsilon_1-1} |_2^2 )</td>
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<tr>
<td><strong>6:</strong> Increase ( \epsilon_1 )</td>
</tr>
<tr>
<td><strong>7:</strong> end</td>
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In order to decrease the effect of noise and impose smoothness as a priori information for more accurate results we have implemented two different regularization methods. In the first approach, we have used gradient-based regularization defined as

\[
R_p(\rho) = \lambda_p \| L\rho \|_2^2 \tag{8}
\]
where $\lambda_{\rho}$ is the regularization parameter, the value of which determines the balance between data mismatch and regularization terms; and $L$ is a discrete gradient matrix including all vertical and horizontal derivatives computed as

$$L = \begin{bmatrix} I \otimes L \\ L \otimes I \end{bmatrix}$$

(9)

with $I$ as an identity matrix with the size of $N \times N$ (assuming we are reconstructing images containing $Np = N \times N$ pixels); $\otimes$ is the Kronecker tensor product operator; and $L$ is the $(N - 1) \times N$ derivative matrix

$$L = \begin{bmatrix} -1 & 1 & 0 & 0 & \cdots \\ 0 & -1 & 1 & 0 & \cdots \\ 0 & 0 & -1 & 1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & -1 \end{bmatrix}$$

(10)

In the second approach, we employ the iterative edge-enhancing regularization methods developed in [24]. Here, (7) is solved repeatedly where from one iteration to the next, the regularization is updated in a manner that de-emphasizes the smoothing for locations in the image where edges are suspected. At iteration $\ell$, takes the form

$$R_{\rho,\ell}(\rho) = \lambda_{\rho,\ell}\|D^{(\ell)}L\rho\|_2^2$$

(11)

where $\lambda_{\rho,\ell}$ is the regularization parameter for every iteration, and $D^{(\ell)}$ is a diagonal weighting matrix with elements between zero and one updated at iteration $\ell$. Those diagonal elements closer to one will enforce smoothness to the associated pixels while the values closer to zero indicate that the associated pixels belong to the edge map and should be preserved. The pseudo code for the iterative edge-preserving regularization is given in Table 2.

<table>
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<td>Pseudo code for iterative edge-preserving regularization</td>
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**Inputs:**
- $\rho^{(0)} = I$
- $L$, gradient matrix
- Estimate of $\rho$ for $\ell = 0, 1, \ldots$

1: for iterations $\ell = 1, \ldots$
2: \hspace{0.5cm} Set $v = D^{(\ell)}L\rho_{\ell-1}$
3: \hspace{0.5cm} Normalize $v$ by setting $v \leftarrow v/\|v\|_{\infty}$
4: \hspace{0.5cm} Map $d$ to $[0,1]$ by defining $d := 1 - v.p$
5: \hspace{0.5cm} Define $D = \text{diag}(D)$
6: \hspace{0.5cm} Update $D^{(\ell)} \leftarrow DD^{(\ell-1)}$
7: end

Table 2: Pseudo code for iterative edge-preserving regularization.

Starting with an appropriate initial guess for the density is crucial to the success of the approach. There are a number of ways this could be accomplished. For example, attenuation based CT images have been shown to be useful in this regard [22], however for the limited view problems that interest most in this effort, re-construction of the photoelectric and density from attenuation data is known to be a highly ill-posed prob-
lem. Thus we are motivated to consider an alternate, multi-scale approach. At the first level, a coarse scale representation of the grid and density vector to be recovered is assumed, and a constant density vector is considered as an initial guess to build the system matrix $K(\rho_0, 0)$. The LSQR method is applied to the linear least squares optimization in (7) and the estimated density image at this level is “upscaled” via the Matlab nearest-neighbor interpolation method, and used as an initial guess to build the system matrix at the next finer scale so on and so forth. After a few iterations we achieve a good approximation of density vector in a desired scale size without any prior information about the density image. The block diagram of the multi-scale approach to estimate density with the edge-preserving regularization method is shown in Figure 2. After estimating density, the results can be used for photoelectric reconstruction explained in the next section.

![Figure 2: Block diagram of multi-scale approach. An estimate of density $\rho_{k-1}$ at scale $k-1$ first resized to the current scale $k$, then a new estimation $\rho_k$ at the current scale obtained via density estimation (using the algorithm in Table 1) and edge preserving regularization (using the method in Table 2).](image)

**C.2. Photoelectric Reconstruction**

Having the density image estimated at hand, we modify equation (6) to reconstruct photoelectric image as the following

$$\hat{p} = \arg\min_p \|g - K(\rho_0, p)\rho_0\|_2^2 + R_p(p)$$

(12)

where $\rho_0$ is the final estimate of density image as a solution to (7) and $R_p(p)$ is the photoelectric regularization. To date we have used the same regularization methods explained earlier for density. We note that, in contrast to the density problem, photoelectric recovery is a non-linear least squares optimization problem which we solved using the Levenberg-Marquardt method [25]. The approach requires the Jacobian matrix of the objective function with respect to $p$ the calculation of which is facilitated by rewriting (12) as

$$F(p) = \|g - K(p = \rho_0, p)\rho_0\|_2^2 + R_p(p) = f(p)^Tf(p)$$

(13)

where $f(p)=[f_m(p); f_r(p)]$ includes the data mismatch and regularization terms given as

$$f_m(p) = g - K(p = \rho_0, p)\rho_0$$

(14)
The Jacobian matrix can be derived analytically by calculating first derivative of $f_m(p)$ and $f_r(p)$ as

$$J = \begin{bmatrix} \frac{\partial f_m(p)}{\partial p} & \frac{\partial f_r(p)}{\partial p} \end{bmatrix}$$

with

$$\frac{\partial f_r(p)}{\partial p} = \sqrt{\lambda_p L}$$

for the first regularization scheme. With $f_{r,\beta}(p) = \sqrt{\lambda_{p,\beta} b^{(\beta)}_p L}$ the Jacobian elements for the second are

$$\frac{\partial f_{r,\beta}(p)}{\partial p} = \sqrt{\lambda_{p,\beta} b^{(\beta)}_p L}$$

For the data mismatch term, the $j$th row of the Jacobian matrix associated with the forward model is

$$\begin{bmatrix} \partial f_{m}(p) \\ \partial f_{r}(p) \end{bmatrix}_j = \begin{bmatrix} \partial f_{m}(p) \\ \partial f_{r}(p) \end{bmatrix}_j$$

$$= \frac{\partial(\int I_0(E_S) \int h(r', E') S(r, \theta, E) h(r, r_E, E_S) l_{r, r_E} (r) \rho_0 (r) dr) dE_S}{\partial p}$$

$$= \int I_0(E_S) \left[ \int \frac{\partial(\int h(r', E') S(r, \theta, E) h(r, r_E, E_S) l_{r, r_E} (r) \rho_0 (r) dr)}{\partial p} dE_S \right]_j$$

where $j \in \{1, \ldots, N_{\text{scat}}\}$ indexes the number of rows in the forward model and Jacobian matrices. The total number of scattered raypaths $N_{\text{scat}} = N_S \times N_D \times (N_D - 1)$, is defined by the number of sources and detectors, $N_S$ and $N_D$, over which absorption data will be collected. Based on (18) the Jacobian matrix requires the computation of the first derivative of the attenuation coefficients for each broken raypath as

$$\frac{\partial h(r', E')}{\partial p} = \frac{\partial(\exp(-\int \mu(r', E') l_{r, r'} (r') dr' - \int \mu(r', E_S) l_{\text{trr}} (r') dr'))}{\partial p}$$

$$= \frac{\partial(\exp(-\int \mu(r', E') l_{r, r'} (r') dr' - \int \mu(r', E_S) l_{\text{trr}} (r') dr'))}{\partial p}$$

$$= \left( -E_S^{-3} \int l_{r, r'} (r') dr' - E'^{-3} \int l_{\text{trr}} (r') dr' \right) \times$$

$$\exp \left( -\int \mu(r', E') l_{r, r'} (r') dr' - \int \mu(r', E_S) l_{\text{trr}} (r') dr' \right)$$

C.3. Results

To evaluate the results of our proposed method we have defined a system setup similar to the system shown in Figure 1. We have considered a discretized area of $50 \text{cm} \times 50 \text{cm}$ surrounded by 3 sources and 41 detectors. Sources are located on the middle of left edge, middle bottom edge and left bottom corner of the grid. Detectors are aligned on the right edge, top edge equally, and the remaining detector is located on the top-right corner of the grid. For each source we have used a normalized source spectrum as shown in Figure 3 (on the next page). Data from 20 - 40 KeV with the step size of 1 KeV is considered for photoelectric recovery, while a wider range of energies from 20 - 120 KeV with the equal step size is used for density reconstruction. In order to consider measurement and discretization noise, a signal-to-noise (SNR) ratio of 50 dB is assumed for the measured scattering data. We have generated a simple phantom consisting of an object at the middle of the grid as shown in Figure 4. The object consists of water with the density of $\rho = 1 \text{ Kg/cm}^3$ and photoelectric...
absorption coefficient of $p = 0.5439\text{cm}^{-1}$ at the energy level of $E_0 = 20\text{ KeV}$ [26].

The multi-scale approach is applied to the phantom with both regularization methods to recover density image and the results are shown in Figure 5 (on the next page). The initial guess is chosen to be a constant background image with the value of $\rho_0 = 0.1\text{ Kg/cm}^3$. The final estimate of density at each scale is demonstrated starting from the grid with the size of $10 \times 10$, and ending with the grid of the size of $50 \times 50$. Figure 5a represents the reconstruction of density of the phantom applying the first regularization method, while Figure 5b shows estimation of density with the iterative regularization method. As predicted, the edge-preserving results obtain more of the structure of the object and leads to a superior result at the final scale. Specifically, the streaking artifacts are significantly reduced, and as expected, the edge of the object is much better defined. Still, the “northeast” edge remains blurry due to the restriction of sources only along the left and bottom edges. In order to estimate photoelectric image, we have used a scaled image of the density estimation at the finest level with the scaling parameter of $p_0 = 3\times \rho_{\text{total}}$. Photoelectric reconstruction results are shown in Figure 6 also for both regularization methods. Final results suggest that the scattering physical model is successful to reconstruct both photoelectric and density characteristic of the material. We feel that work remains in terms of optimal regularization for improving the photoelectric reconstruction.

Both regularization parameters for density and photoelectric, $\lambda_\rho$ and $\lambda_p$, are selected in a similar approach. In the first iteration, we have performed a greedy search on a logarithmic scale in the range of $[10^{-4}...10^{10}]$ for the regularization parameters. To find the optimal regularization parameters, we assume that the real phantom is known, and the parameter which gives the minimum least square error is selected as the optimum value. As we discuss below, lifting this assumption is an issue that needs to be addressed in the coming year. Further, we have narrowed down the range of our greedy search for the next iteration around the optimum value obtained in the previous step.

![Figure 3: Normalized source energy spectrum.](image)

Figure 4: Original phantom. A simple circle-shaped object consisted of water with the radius of 20 cm is considered. The density and photoelectric absorption coefficients are $\rho = 1\text{ Kg/cm}^3$, $p = 0.5439\text{cm}^{-1}$ at $E_0 = 20\text{ KeV}$ respectively.
Figure 5: Reconstruction results for density image at 5 different scales. The grid size at the first scale is $10 \times 10$ and increasing at every dimension by 10 where the finest grid size at the last level is $50 \times 50$. The area of the grid is $50 \text{cm} \times 50 \text{cm}$ and the density values are $0 - 1 \text{ Kg/cm}^3$. Left column (a) illustrates the estimation results using the first regularization method, and the right column (b) shows the estimation results using the edge-preserving regularization method.
C.4. Related Work: Multi-energy sinogram decomposition

As mentioned in the introduction, we have also been pursuing research related to processing of transmission X-ray data acquired using energy-resolving detectors. The same detectors that support Compton scatter tomography (by giving information on energy transfer), also allow potentially improved processing of transmission data.

As background, there is growing interest in developing X-ray computed tomography (CT) imaging systems with improved ability to discriminate material types, going beyond the attenuation imaging provided by most current systems. Dual-energy CT (DECT) systems can partially address this problem by estimating Compton and photoelectric (PE) coefficients of the materials being imaged, but DECT is greatly degraded by the presence of metal or other materials with high attenuation. Here we explore the advantages of multi-energy CT (MECT) systems based on photon-counting detectors. The utility of MECT has been demonstrated in medical applications where photon-counting detectors allow for the resolution of absorption K-edges. Our primary concern is aviation security applications where K-edges are rare. We simulate phantoms with differing amounts of metal (high, medium, and low attenuation), both for switched-source DECT and MECT systems, and include a realistic model of detector energy resolution.

As a first contribution, we extended the DECT sinogram decomposition method of Ying et al. [31] to MECT, allowing estimation of separate Compton and photoelectric sinograms. We furthermore introduced a weighting based on a quadratic approximation to the Poisson likelihood function that deemphasizes energy bins with low signal. Similar to previous dual-energy work, we model the attenuation through the object in terms of Compton and photoelectric coefficients, as these are the dominant attenuation mechanisms in the energy range of interest. Thus, our forward model for the $i^{th}$ raypath becomes:

$$K(\theta^i) = \ln \left( \frac{\int S(E) \exp(-\lambda_i f_{\text{Kx}}(E)-\lambda_p f_p(E)) dE}{\int S(E) dE} \right)^{\frac{1}{\theta^i}}$$  \hspace{1cm} (20)$$

This model can then be used in an inverse problem in which we seem to minimize the difference between the forward model and the measurements. While the underlying statistics are Gaussian, we have shown good results using a quadratic approximation to the Gaussian, namely,
where $m_i$ are the vector of multi-energy measurements for all energy bins on raypath $i$. The weighting matrix $\Sigma$ is a diagonal matrix whose diagonals contain the number of counts for each energy bin \([31]\). Thus, bins with higher counts (less attenuation) are more highly weighted than low-count bins. This weighting is the primary difference between a standard least-squares approach and the one we propose, and as documented in our results, leads to noticeable performance gains.

Simulation results, shown below, compare the proposed approach to a standard switched dual-energy method. In this example, the center object is aluminum, so most ray paths are highly attenuated. As a result, substantial artifacts are seen in the dual-energy (DECT) approach, whereas the multi-energy method essentially recovers ground truth very closely. Benefits are smaller, but less noticeable, when the aluminum is replaced by a lower-attenuation material, or a smaller (less attenuating) aluminum object is used. In this example, the proposed approach improves the signal to noise ratio of reconstructions by over 20 dB.

\[
\log P(m^i|\theta^i) \approx -\frac{1}{2} (K(\theta^i) - m^i)^T \Sigma^i (K(\theta^i) - m^i) + c(m^i) \tag{21}
\]

Figure 7: Reconstruction results (assuming good angular spacing, and use of inverse Radon transform) for switched dual-energy (top row) vs. weighted multi-energy processing. Because of the large amount of metal in the phantom, significant artifacts are seen in the dual-energy case, which are avoided in the multi-energy result.

An important question is whether this performance improvement is particular to the algorithms used, or is a general feature of multi- vs. dual energy sinogram decomposition. To numerically evaluate the performance of the weighting based MECT, the Cramer-Rao lower bound (CRLB) is employed to determine the upper bound of signal-to-noise ratio (SNR) for both Compton and PE coefficients in the sinogram domain. A prominent improvement can be seen by using MECT compared to the conventional switched-source DECT. The upper bound eventually converges as the number of energy bins approaches 5-10. This result supports the conclusion that multi-energy detectors provide additional useful information, and also suggests that
even fairly coarse energy resolution (which may allow use of cheaper detectors) may be sufficient to achieve performance gains.

![Figure 8: Cramer-Rao bounds on SNR for both less-attenuating (nylon) and more attenuating (aluminum) materials, for a variety of material thicknesses. As can be observed, the theoretically obtainable SNR increases as the number of energy bins increases, but asymptotes before 10. Dashed curves show the obtainable results for a traditional switched dual-energy system (which because of the spectrum overlay typical in these systems, underperforms the multi-energy detectors even for the case of two energies).](image)

Finally, we have prepared code for processing data that we anticipate will be collected under the 13.05 effort. Improved sinogram reconstruction, especially in the presence of metal, has the potential for reducing false alarms in checkpoint and checked baggage inspection, and is a potential transition opportunity for our work.

### D. Major Contributions

- **Phase 2, Year 3:** We have demonstrated a method for joint recovery of both density as well as photoelectric coefficient from severely limited view, multi-energy Compton scatter data. The overall approach is based on a variational formulation of the imaging problem. Physical intuition has guided the specific method used to solve this problem. Initial results on simulated data are quite promising.

- **Phase 2, Year 2:** We have developed a tractable, analytical model capable for X-ray scattering and attenuation. The model has been instantiated in the form of a Matlab-based code that will be made accessible to the broader DHS community. We believe that the model can be used effectively and efficiently in the context of image reconstruction methods seeking to recover spatial maps of electron density and photo-electric absorption information from limited view, multi-energy X-ray data.

- **Phase 2, Year 1:** Our initial efforts under Phase 2 of ALERT support were the development of a computational forward model for multi-energy, limited view X-ray scanner modeled on the AS&E CANSCAN system, the limited view system which is to form the basis for the 13-05 project. At the start of Phase 2, Year 2, we decided to move away from this absorption-only model as we began to explore the potential for scattered photon data to address the many challenges associated with the processing of limited view information.

### E. Milestones

The two milestones identified in the Year 3 project report were:
1. The development of variationally-based image formation algorithms. This milestone was accomplished. An overview of the processing approach has been provided in the previous portions of this section of this report.

2. The validation of image formation algorithms based on data collected by AS&E under our 13-05 effort. The time-line of the 13-05 project has been such that the system to collect the data is, as of the writing of this report, still under construction. We anticipate that the system will be completed during the summer of 2016 and initial data collected. That data will be used to validate both the forward model as well as the image formation methods.

The work in Year 4 will focus on achieving the following three milestones:

1. Improvements to the current processing scheme.
2. An evaluation of the current method on more complex simulation data as well as real data generated under our 13-05 effort.
3. An extension of the processing methods. More specifically, based on our multi-energy, limited view CT work over the past seven years, we anticipate that more complex scenarios will result in the loss of some performance of the current method for recovering the photoelectric coefficient.

F. Future Plans

Our plans for the coming year will focus on achieving the two milestones identified at the end of the last subsection. In terms of the current approach to processing, the one area that needs to be improved is the selection of the regularization parameters, $\lambda_\rho$ and $\lambda_p$, used to balance the influence of the three terms in the cost function. To date, we have been choosing the “optimal” values for these parameters assuming we knew the true images. Clearly, this is not realistic. Well-established methods exist in the literature for selecting these quantities including the discrepancy principle [27, Chapter 7] and the so-called L-surface [28]. Both will be considered in the coming year.

We will explore two strategies for addressing the challenges posed by real data and complex imaging scenarios.

1. First, we shall augment the Compton scatter data with energy-resolved attenuation data. Indeed, the AS&E system will in fact collect both classes of data. Essentially, the effort here is one of data fusion. We believe it will be complicated by certain characteristics of the two different types of data. While the number of scatter data will be high (many source-detector pairs), the signal to noise ratio i.e., the number of counts, in each may be relatively low. On the other hand, the number of attenuation source-detector paths will be smaller than those due to scatter but the number of counts, and hence the quality of the signal will be larger. One issue we anticipate facing is how best to weigh these two sources of data in the variational image recovery method to ensure that we make “optimal” use of the information in each. Here we will be guided by ideas in [29] where a data fusion inverse problem with similar characteristics was considered in the context of a geophysics application.

2. The second strategy will focus on the development of appropriate regularization strategies for stabilizing the recovery specifically of the photo-electric coefficient. Our initial approach here will be motivated by our prior efforts in multi-energy CT. In [30], we developed a patch-based scheme which exploited the fact that we could stably recover Compton scattering maps to help improve the photo-electric images. We believe there may be merit in further development and application of the idea to stably recover the photoelectric map.

The ability to estimate the photoelectric coefficient in a stable manner is the major risk to this project. Our mitigation strategy then is the anticipated need to apply and adapt existing regularization methods we have developed in the X-ray CT context to the Compton scatter case of interest here.
We anticipate that the project will conclude by the end of Year 5. The major task to be accomplished in this last year is related to metal artifact reduction. Our original motivation for exploring scatter tomography was to help with reducing imaging artifacts caused by presence of metal in the scene. Over the fifth and last year of this project, we propose to combine the Compton scatter processing methods developed to date with our prior geometric inversion methods in an effort to identify directly the geometry of metallic objects. This alternative to a pixel-based reconstruction should further stabilize our ability to recover photoelectric maps, reduce artifacts in the images, and allow for accurate recovery of material properties for objects located adjacent to metals.

III. RELEVANCE AND TRANSITION

A. Relevance of Research to the DHS Enterprise

We are seeking to address challenges associated with automated scanning and threat detection in both checked luggage and baggage that are inspected at checkpoints. The overall goal is to determine spatial maps of material properties in an automated manner from multi-energy X-ray data collected in limited-view types of geometries characteristic of many systems currently under development by DHS contractors. The results of these efforts will be a reduction in the false alarm rate of these systems, along with increased accuracy in the localization and characterization (size, shape, material type) of threat objects. Any metric that quantifies the accuracy of the material maps can be used to evaluate the performance of our work including:

- Confusion matrices capturing the percentage of correctly and incorrectly labeled pixels for scenarios where ground truth is known.
- If one is concerned with purely binary problems (threat object versus all other types of materials), then that receiver operating curve’s plotting detection probabilities versus false alarm measures could be developed.
- Finally, we could visualize accuracy using uncertainty cloud analysis developed as part of ALERT Task Order 3 and employed in [26]. These clouds would plot the average value and first standard deviation ellipse of the distribution of photoelectric and electron density over known target regions in our reconstructions. In comparing multiple candidate processing methods, smaller ellipses and means closer to ground truth are indicators of higher accuracy.

B. Potential for Transition

As indicated previously in this document, the Tufts University group being supported by ALERT is also teamed with American Science and Engineering (AS&E) on a 13-05 project that is focused on constructing a system designed specifically to implement the processing methods being developed in this project. As this AS&E 13-05-based system embodies the physical models and image formation methods whose development was funded by ALERT, it represents our primary transition product. In addition, we are committed to releasing all codes to the broader user community via any process established by the ALERT center. In addition to this 13-05 effort that will be on-going over Year 4, we plan on engaging the user community through our attendance and participation in ADSA workshops, and the 4th International Conference on Image Formation in X-Ray Computed Tomography in Germany, as well as the replacement for the Gordon Research Conference on explosives detection.

C. Data and/or IP Acquisition Strategy

As noted above, data will be acquired under the 13-05 effort involving Tufts University and AS&E (lead) to validate and refine the methods being developed under support from ALERT. Any Intellectual Property developed during the effort will be disclosed via the patent process if the importance of the IP warrants.


D.  Transition Pathway

In addition to the collaboration with AS&E, the team at Tufts University is very willing to present the work discussed in this report at future ADSA meetings. In addition, Professors Miller and Tracey have engaged in discussions with both Analogic and Rapiscan concerning collaboration on X-ray imaging algorithms. While these discussions have not as yet yielded the same level of engagement as the AS&E collaboration, we are always willing and interested in pursuing transition activities.

E.  Customer, User, and/or Commercialization Partner Connections

See response above.

IV. PROJECT ACCOMPLISHMENTS AND DOCUMENTATION

A.  Education and Workforce Development Activities

1.  Other Outcomes that Relate to Educational Improvement or Workforce Development
   a.  Ms. Hamideh Rezaee, is currently pursuing her PhD in Electrical and Computer Engineering at Tufts under full support from ALERT. This project has provided her with a special educational opportunity to engage in fundamental research on a problem that is of intense interest to a wide range of people. As Professors Miller and Tracey have worked with Dr. Couture from AS&E to plan for 13-05, her effort on multi-energy Compton scatter reconstruction has proven to be central to this collaboration. In the remaining years of her PhD studies, Ms. Rezaee will be provided with a rather unique experience where the results of her efforts will be directly translated to our industrial partner; and via the ADSA workshops, disseminated to a broader community of researchers from academia, corporate labs and the government.

B.  Peer Reviewed Journal Articles


C.  Peer Reviewed Conference Proceedings


D.  Other Conference Proceedings

E. Student Theses or Dissertations Produced from This Project


F. Software Developed

1. Other
   a. We have developed a fully commented Matlab code and associated user manual implementing the absorption and scattering model described in this report. We will work with the ALERT administration to determine how it can be distributed to the community.

V. REFERENCES


