

# Hyperspectral Neutron CT with Material Decomposition



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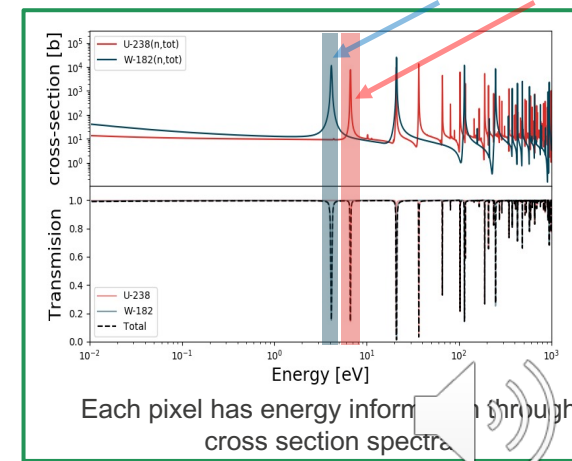
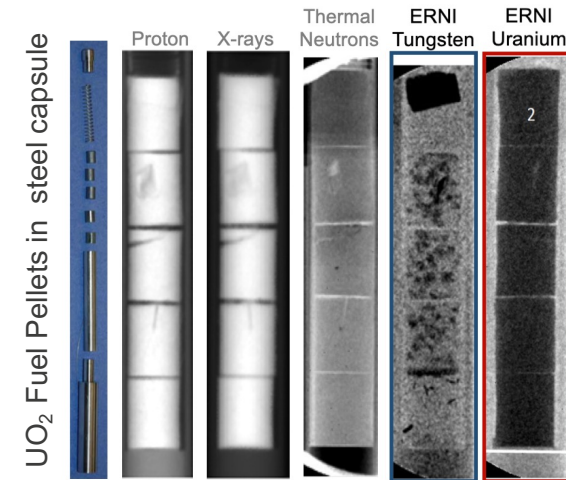
<sup>2</sup>Los Alamos National Laboratory



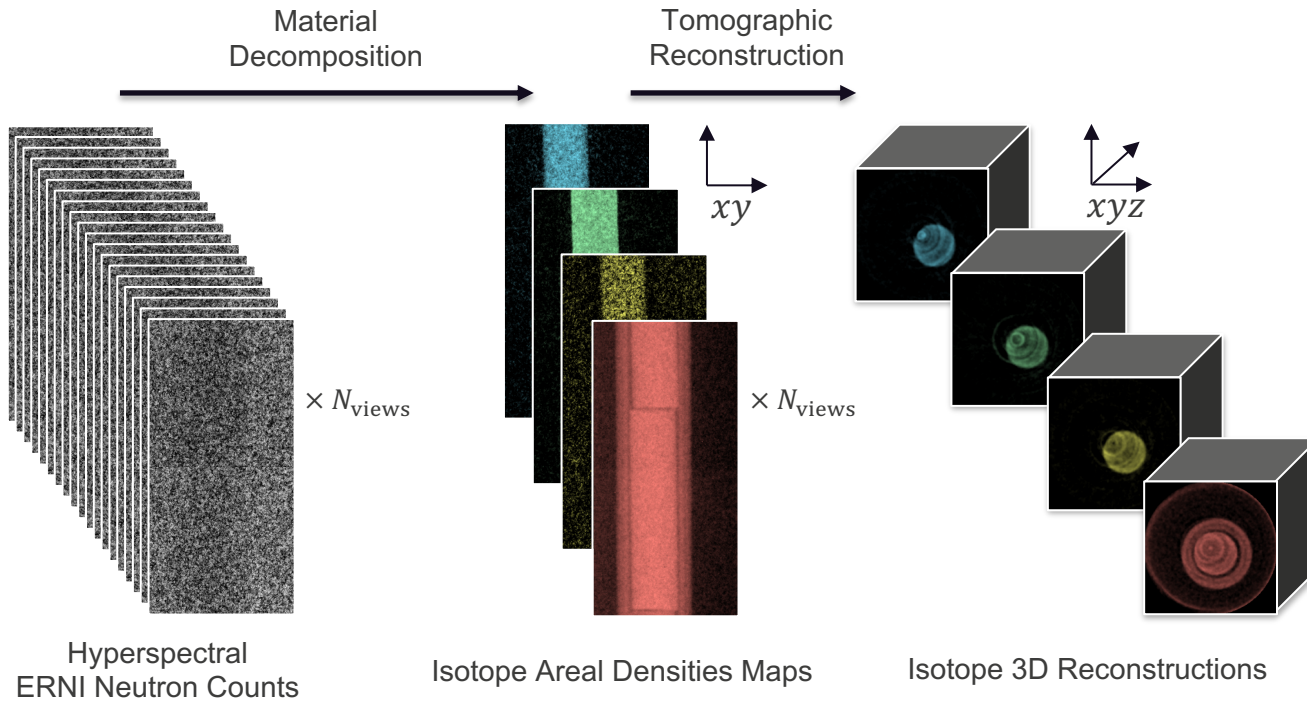
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# ERNI (Energy Resolved Neutron Imaging)

- Neutron radiography fundamentally different contrast mechanism than x-rays or protons:  
*nuclear interaction vs. electron shell*
- Much higher penetration for most materials than typical x-ray sources but sensitivity to hydrogen
- Short pulsed neutron sources allow for energy resolved neutron imaging through the time-of-flight (TOF) technique
- Cross section resonances in epithermal energy act as *unique fingerprints*



# Overview



# Main Challenges

## Extreme Noise

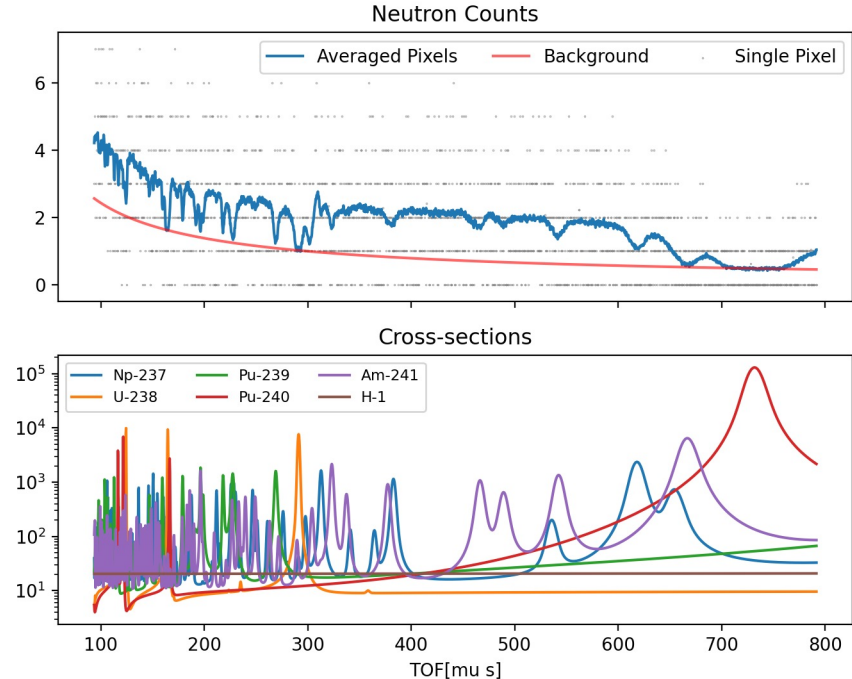
- Very low counts even with months of scan time
- Background counts are significant, random and unknown

## Large data size

- Hyperspectral feature adds degree of freedom
  - Easily 100s GB to 100s of TB
- *Several months of processing time* with nuclear analysis tool SAMMY (state-of-the-art)

## Measurement system partly unknown

- Background counts unknown
- Unknown resolution blurring breaks Beer's Law
- Inaccurate isotope cross section spectra



# Measurement Model

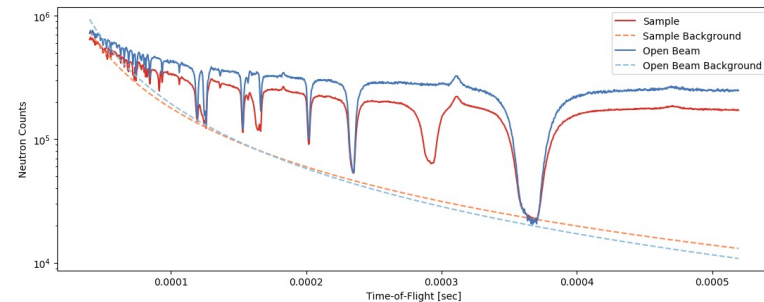
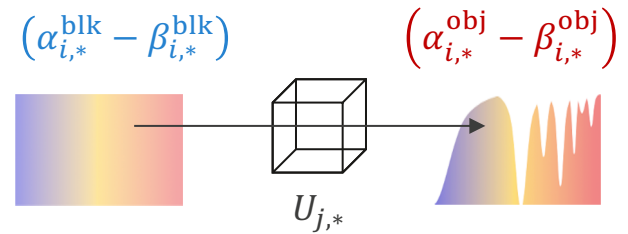
- Neutron count measurements consists of
  - Blank scan  $\alpha^{\text{blk}}$
  - Object scan  $\alpha^{\text{obj}}$ ,
 resolved in energy bins,  $k$ , and projection index,  $i$ .
- Total counts,  $\alpha$ , have significant background,  $\beta$ .
- Each voxel,  $j$ , has an attenuation spectrum,  $U_{j,*}$

$$\frac{\alpha^{\text{obj}} - \beta^{\text{obj}}}{\alpha^{\text{blk}} - \beta^{\text{blk}}} = T = \exp(-Y) = \exp(-AU) + \text{noise}$$

Transmission measurement

Attenuation Densities

- Finding hyperspectral densities,  $U$ , directly is impractical:
  - Neutron counts extremely noisy
    - Independent CT's impractical
  - Data set extremely large due to 1000s of energy bins
    - Joint CT's impractical
- We are interested in the material composition

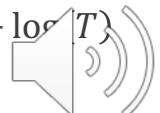


$T$ : Transmission Measurement

$U$ : Attenuation Density

$A$ : Tomographic System Matrix

$Y$ : Attenuation Measurement =  $-\log(T)$

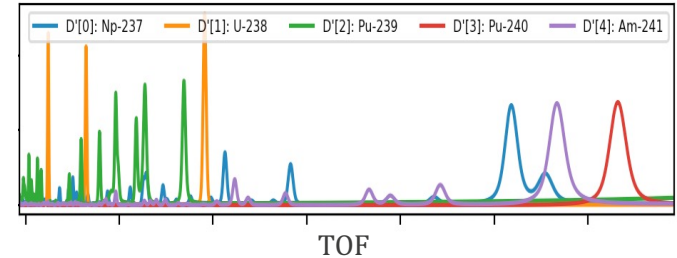


# Reduction of Dimensionality

Isotopes have known attenuation spectra, **cross sections**,  $\sigma$   
 Beer-Lambert law relates transmission with **areal densities**,  $\rho_i$

$$-\log(T) = Y = \sum_{i=1}^{N_m} \rho_i \sigma_i + \text{noise} = ZD + \text{noise}$$

$\sqrt{\text{Cross Sections}} = \sqrt{D}$



$$U = XD \rightarrow$$

**Forward Model**

$$Y = AU + \text{noise}$$

$$Y = AXD + \text{noise}$$

Solve for "AX"  $\Rightarrow \hat{Z}$

Solve for X  $\Rightarrow \hat{X}$

Neutron Count  
 Measurements  
 $\alpha^{\text{obj}}, \alpha^{\text{blk}}$

**0. Background Estimation**

$$Y = -\log\left(\frac{\alpha^{\text{obj}} - \beta^{\text{obj}}}{\alpha^{\text{blk}} - \beta^{\text{blk}}}\right)$$

Y: Attenuation Measurements

Y

**1. Material Decomposition**

Reduce Dimensionality

$$Y = ZD + \text{noise}$$

Z: Areal Density Maps

$\hat{Z}$

**2. Tomographic  
 Reconstruction**

$$\hat{Z} = AX + \text{noise}'$$

X: Material Decomposed



# Background Estimation using Opaque Resonances

**Background** := counts that arrive in an energy bin,  $E$ , that are not neutrons of energy,  $E$ .

At opaque resonances of the sample,  $\alpha = \beta$ , so the counts equal the background

## Our Approach:

Find background as maximum lower bound of the counts and smooth in log-log.

$$\tilde{t} = \log(t), \quad \tilde{\alpha} = \log(\alpha), \quad \tilde{\beta} = \log(\beta)$$

(TOF-vector)

Functional for background:

$$\sum_{i=0}^k \tilde{t}^i x_i = G(\tilde{t})x \quad (\text{polynomial})$$

Maximize Area:

$$\int_{t_1}^{t_N} G(\tilde{t})x \, d\tilde{t} = \sum_{i=0}^k x_i \frac{1}{i+1} (\tilde{t}_N^{i+1} - \tilde{t}_1^{i+1}) = -c^T x$$

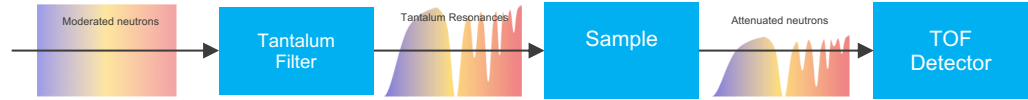
Constraint:

$$G(\tilde{t})x \leq \tilde{\alpha}$$

Linear Programming formulation:  $\hat{x} = \arg \min_x \{c^T x\}, \quad \beta = \exp(G(\tilde{t})\hat{x})$

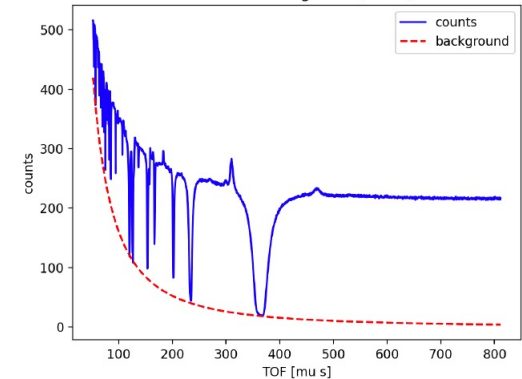
$$G(\tilde{t})x \leq \tilde{\alpha}$$

For individual pixels with high noise counts, background is determined as scaled version of reference background using transparent energy region as reference.

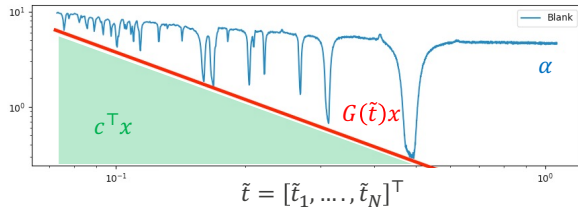
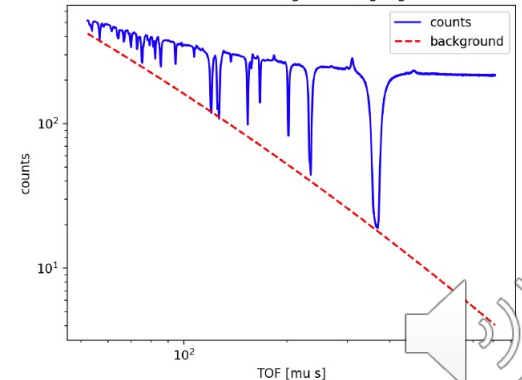


Helps estimate background through opaque resonances

Counts vs. Background (linear)



Counts vs. Background (log-log)



$$\tilde{t} = [\tilde{t}_1, \dots, \tilde{t}_N]^T$$

# Material Decomposition: Solving $Y = ZD + \text{noise}$

## Noise Modeling:

Attenuation,  $Y$ , random with unconventional distribution

$$Y = -\log\left(\frac{\alpha^{\text{obj}} - \beta^{\text{obj}}}{\alpha^{\text{blk}} - \beta^{\text{blk}}}\right), \quad \alpha\text{'s and } \beta\text{'s are Poisson}$$
$$\text{Var}(Y|Z) \approx \frac{\alpha^{\text{obj}} + \beta^{\text{obj}}}{(\alpha^{\text{obj}} - \beta^{\text{obj}})^2} + \frac{\alpha^{\text{blk}} + \beta^{\text{blk}}}{(\alpha^{\text{blk}} - \beta^{\text{blk}})^2} = V^{-1}$$

Gaussian approximation for negative log-likelihood:

$$-\log \mathbb{P}(Y|Z) \approx \frac{1}{2} \|D^T Z^T - Y\|_V^2$$

## Reconstruction:

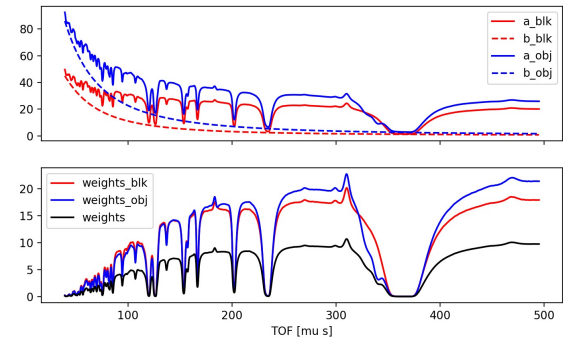
Compute decomposed sinogram,  $Z$ , as maximum a posteriori (MAP) estimate using Basis Pursuit Denoising (BPDN):

$$\hat{Z} = \arg \min_{Z \geq 0} \left\{ \frac{1}{2} \|D^T Z^T - Y\|_V^2 + \rho \|Z^T\|_1 \right\}.$$

*The objective is separable by projections, so we solve it one view at a time!*

$Y$ : Hyperspectral attenuation measurement  
 $Z$ : Areal density maps  
 $D$ : Dictionary of cross sections

Counts and inverse variances (weights)



$\alpha^{\text{blk}}, \beta^{\text{blk}}$   
 $\alpha^{\text{obj}}, \beta^{\text{obj}}$

$V$





# Tomographic Reconstruction: Solving $\hat{Z} = AX + \text{noise}'$

$$\hat{Z} = AX + \text{noise}'$$

Hyperspectral sinogram:

$$\text{Cov}(Y_{i,*}|Z)^{-1} = V_i \quad (N_{\text{energy}} \times N_{\text{energy}} \text{ diagonal})$$

Decomposed sinogram:

$$\text{Cov}(\hat{Z}_{i,*}|X)^{-1} \approx (D^+)^T V_i D^+ = W_i \quad (N_{\text{material}} \times N_{\text{material}} \text{ dense})$$

$$-\log \mathbb{P}(\hat{Z}|X) = \frac{1}{2} \sum_i \|\hat{Z}_{i,*} - A_{i,*}X\|_{W_i}^2$$

Impractical since  $W_i$ 's are dense precision matrices

Since the cross sections,  $D$ , are approximately orthogonal, use

diagonal approximation:  $(W^{(m)})_{i,i} = (W_i)_{m,m}$

$$-\log \mathbb{P}(Z|X) \approx \frac{1}{2} \sum_{m=1}^{N_{\text{material}}} \|\hat{Z}^{(m)} - AX^{(m)}\|_{W^{(m)}}^2$$

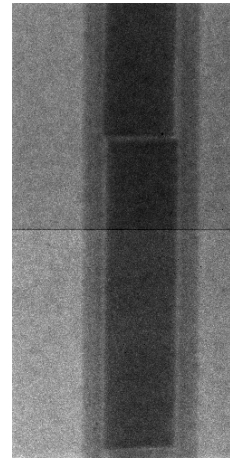
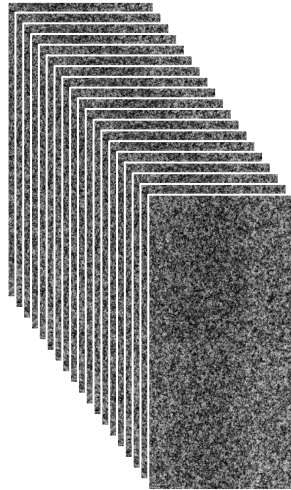
Independent, separable reconstructions using SV-MBIR [1] with q-GGMRF prior model

$\hat{Z}^{(m)}$ : sinogram of material,  $m$   
 $X^{(m)}$ : CT volume of material,  $m$

[1] Xiao Wang, et. al. "High performance model based image reconstruction," SIGPLAN Not., vol. 51, no. 8, Feb. 2016.



# Demonstrating CT on U-Pu-Zr Dataset



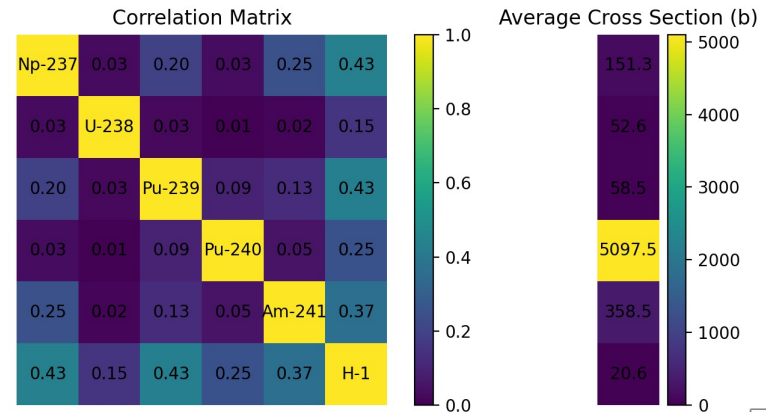
ERNI Data  
100 views, 2290 TOF bins  
each with bin width of 320 ns  
1eV to 60 eV

Acquired at LANCE

Single View  
Averaged over Energy

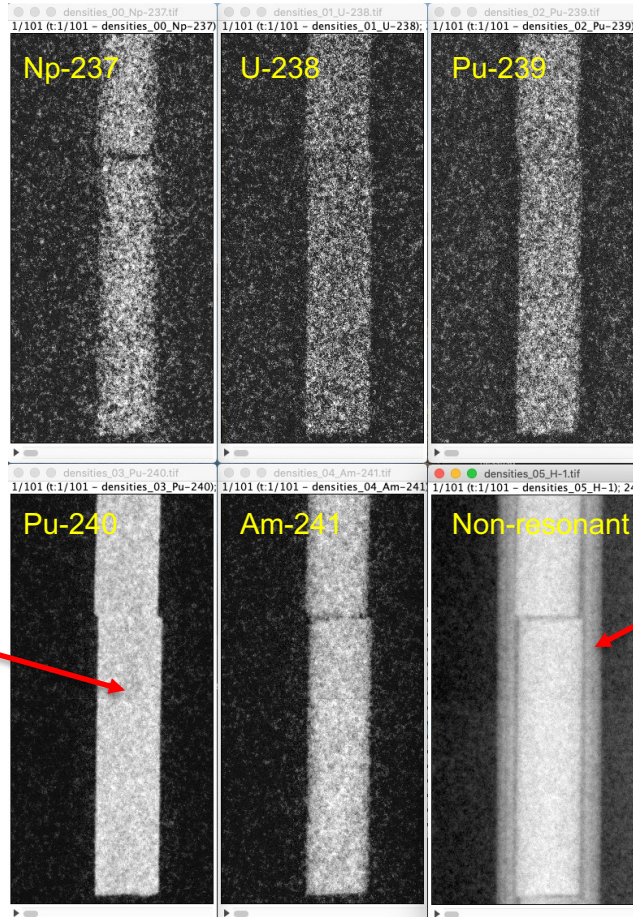
- ERNI CT: U-Pu-Zr Fuel Pellet in Steel Container
- Low correlation of cross section spectra allows for independent CT's

## Cross-section Dictionary



# Material Decomposition Results

Low noise areal density maps,  $\hat{Z}$ ,  
(from high noise ERNI measurement)



Saturation effects from linear model insufficiencies

Steel container and zirconium core component (non-resonant)

Hydrogen (H-1) class  
combines detection of all  
isotopes without distinct  
resonances



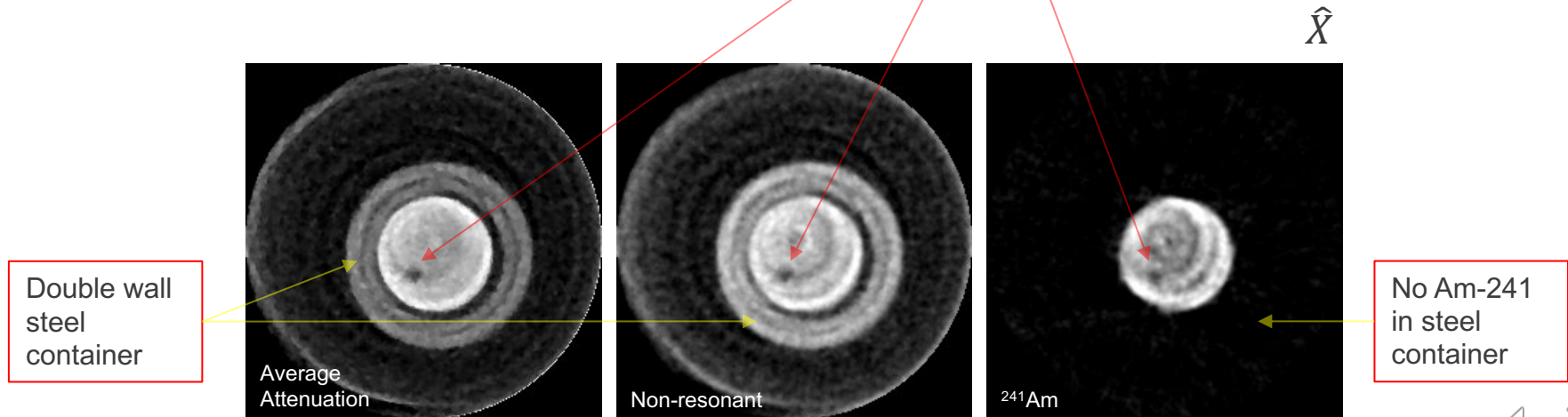
# ERNI-CT Results

Current CT results accomplish to

- Give semi-qualitative measures of isotope distribution
- Allow determining features

Common feature detected,  
guiding destructive evaluation

## Density Maps of 3D CT Reconstruction



# Comparison to SAMMY

**Table 1.** Computation time comparison of the material decomposition. (\*: interpolated, \*\*: extrapolated)

Computation Time	SAMMY	Proposed
Time per pixel spectrum	1.72 s	2.18 ms*
Time per CT data set	248.8 days**	7.58 h

**Table 2.** Estimated Areal densities for a single spectrum. (\* SAMMY did not converge using  $^1\text{H}$ )

Areal Densities [atoms / 1000 barn]	SAMMY	Proposed
$^{237}\text{Np}$	0.471	0.577
$^{238}\text{U}$	10.665	1.163
$^{239}\text{Pu}$	1.930	2.284
$^{240}\text{Pu}$	0.540	0.001
$^{241}\text{Am}$	0.493	0.727
$^1\text{H}$ equivalent	N/A*	0.031

About 800X speedup:  
 **$\approx$  8 months vs 8 hours**

Similar density estimates as SAMMY, with some outliers due to saturation effect.

In future, ground truth data or simulated data necessary to verify accuracy.



# Conclusion and Future Work

- **Conclusion:**

- First full material decomposed neutron TOF CT reconstruction pipeline
- Significant speedup compared to processing with SAMMY
- Robust background estimation
- Material decomposed radiographs possible when CT not available

- **Future/Current Work:**

- Quantitative accuracy not verified
  - Use well defined ground truth phantom, simulated data with Geant4
- Model struggles with saturation effects, noise and finite pulse width
  - Use non-linearized model
  - model Poissons directly
  - model resolution function due to finite pulse width of neutron beam



# Thank you

More questions?

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