Team BIOE21, Triple Helix: **Machine Learning-Based Material Decomposition in Spectral Chest Radiography**

U.S. FOOD & DRUG ADMINISTRATION
BIOCOMPUTATIONAL ENGINEERING

Quentin Molina, Sujay Srinivasan, Braden White

Advisors: Dr. Bahaa Ghammroui PhD, and Harsha Marupudi,
Division of Imaging Diagnostics and Software Reliability, OSEL, FDA

A. JAMES CLARK SCHOOL OF ENGINEERING

Motivation

__Background__:

- More than **70 million** chest radiography exams are performed annually (~20% of all annual radiology exams).
- **Conventional CT scans are often inefficient,** produce variable image quality, and face **limitations** in both reliability and radiation exposure.
- Soft tissue **structures** are **obscured** by high-attenuation bone, limiting detection of ~65% of lung nodules

__Current Solution:__

- **Photon counting computed tomography** allows for both **higher resolution** and **material decomposition.**
- **Photon counting detectors** directly converts X-rays into electrical signals
- Delivers superior resolution with a fraction of the radiation dose.

Objectives

To use **machine learning** techniques to perform **material decomposition** in **spectral chest radiography** simulated with photon-counting detectors (PCD).

Impacts and Ethical Implications

Reduces patient risk: lower radiation exposure

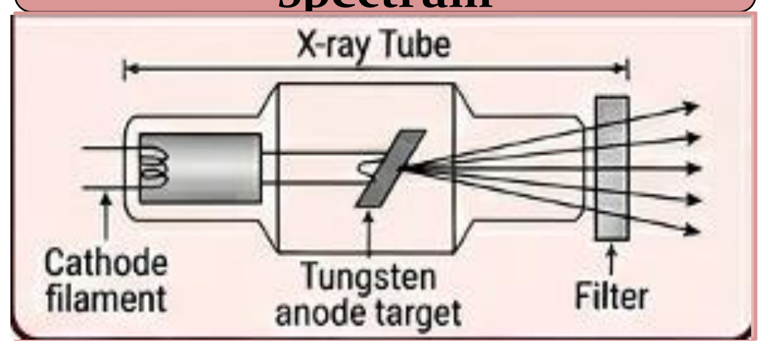
Reduces patient costs: fewer acquisitions translates to reduced medical finances

Enhances resolution: better contrast differentiation

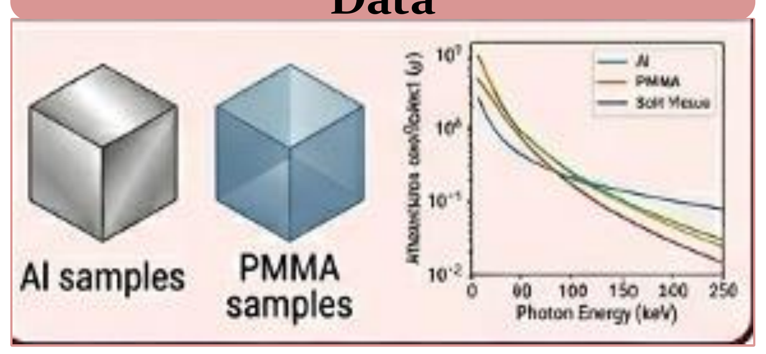
AI ethics: reliability, explainability, and interpretability of AI in regard to AI-assisted workflows

Workflow

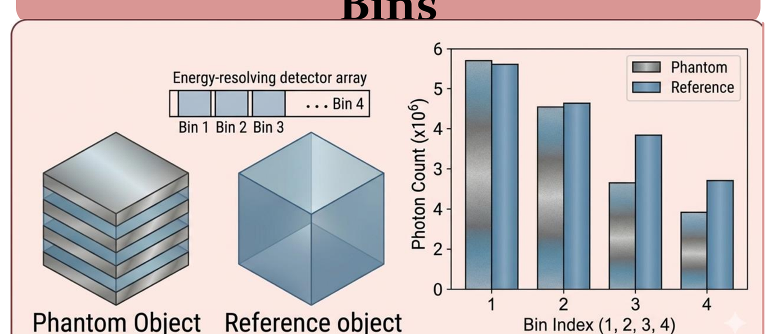
Step 1: Generate X-Ray Spectrum



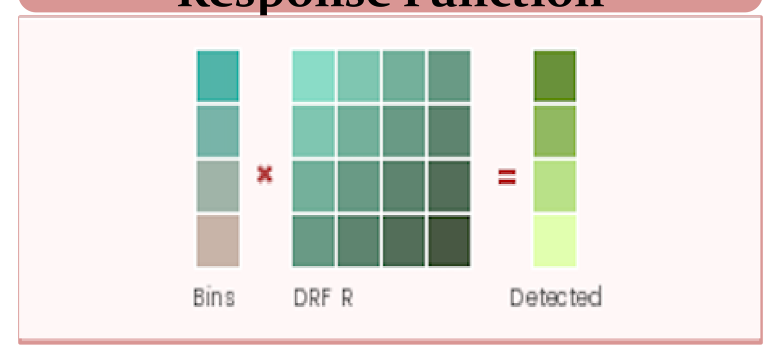
Step 2: NIST XCOM Attenuation Data



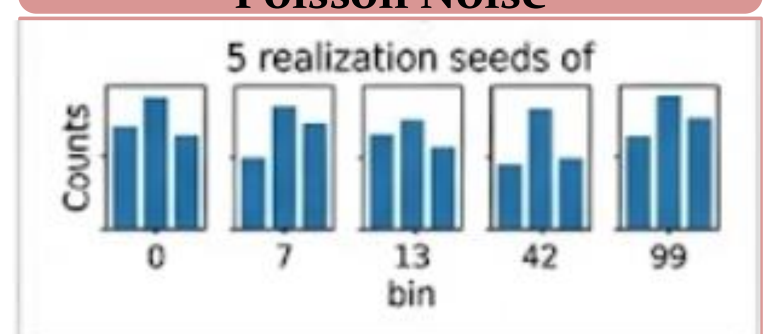
Step 3: Photon Counts & Energy Bins



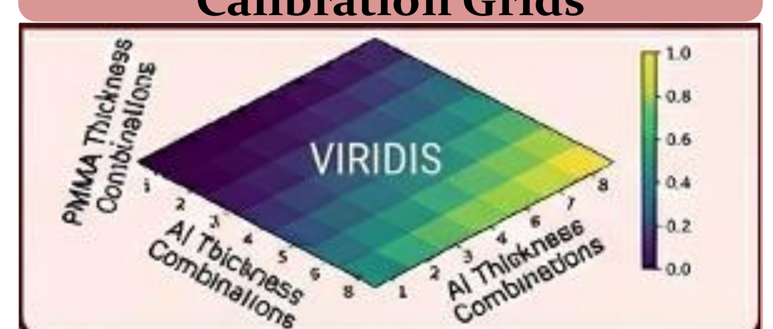
Step 4: Apply Detector Response Function



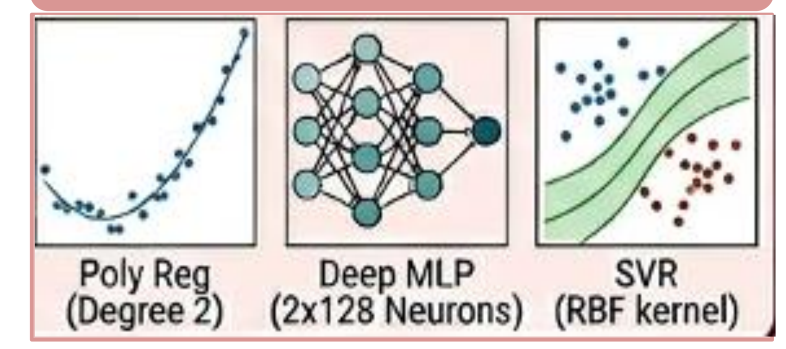
Step 5: Randomly Generate Poisson Noise



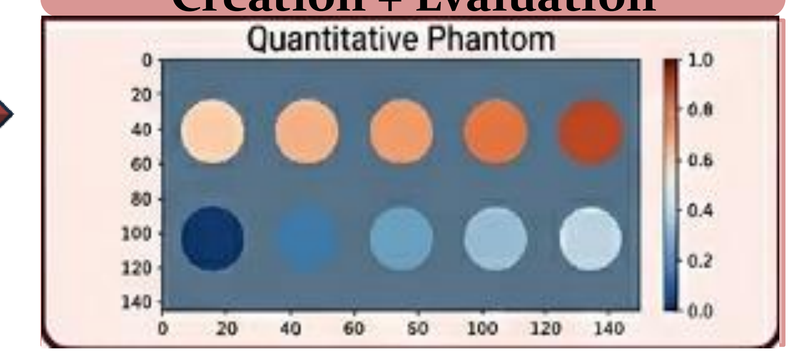
Step 6: Create Thickness Calibration Grids



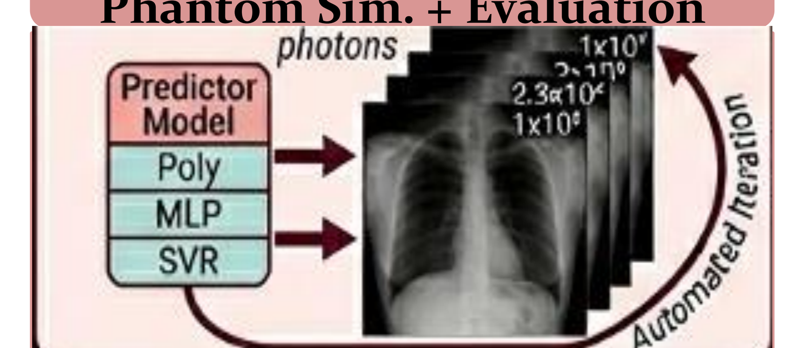
Step 7: Train ML Models



Step 8: Material Phantom Creation + Evaluation



Step 9: Anthropomorphic Phantom Sim. + Evaluation



Conclusions

- Physics-informed **PCCT simulations** with Aluminum and PMMA material phantoms produced **realistic images** and CNR results.
- **Polynomial regression, MLP and SVR** successfully approximate material thicknesses from transmitted polychromatic X-Ray spectrum with low bias and RSME
- MLP models produced **superior material distinctions** for nodule detection in synthetic chest phantoms.

Future Work

- **Refine** pipeline to handle **lower doses** (40-60 keV) more effectively
- **Continue** development into image reconstruction for **3D volumes**
- **Test** pipeline on more complex digital phantoms
- **Translation** to **clinical validation**

Results

Material Phantoms

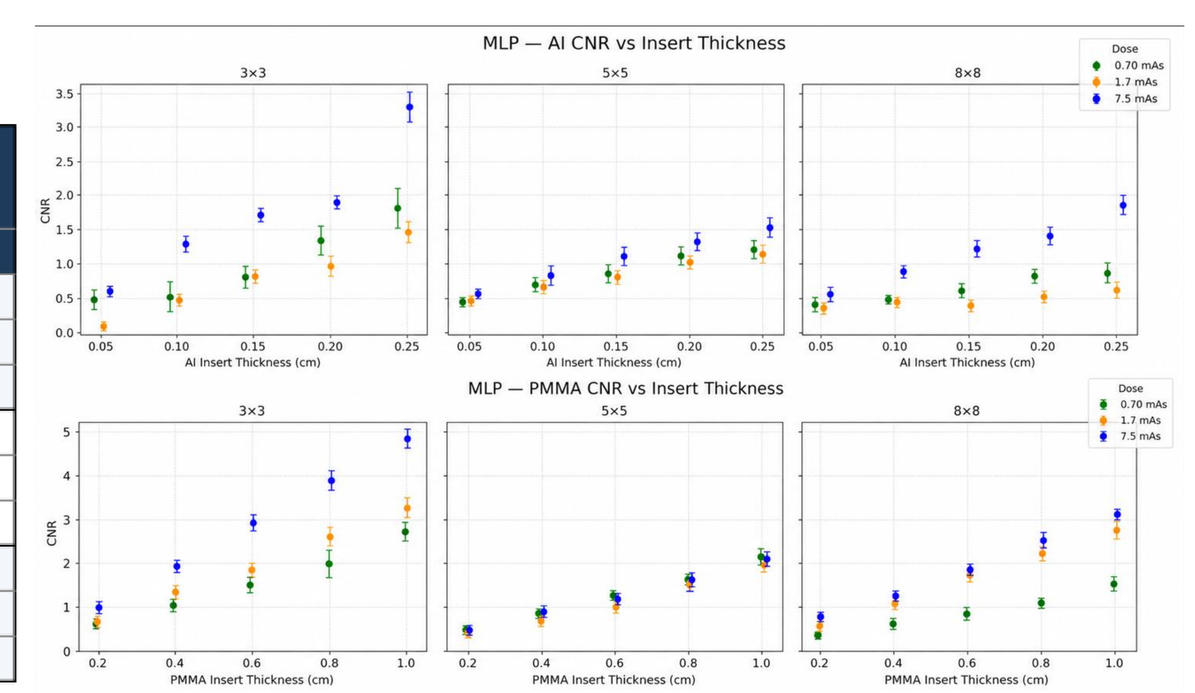
Material Decomposition Accuracy: Al & PMMA Insert Recovery

Mean |bias| / RMSE in cm, averaged over 5 insert thicknesses and 5 Poisson noise realizations

Calibration grid	Method	Low dose ~0.07 mAs (1.0×10^6 ph)		Mid dose ~1.7 mAs (2.3×10^6 ph)		High dose ~7.5 mAs (1.0×10^7 ph)	
		Al insert	PMMA insert	Al insert	PMMA insert	Al insert	PMMA insert
3×3	Polynomial	0.166 / 0.167	0.866 / 0.867	0.528 / 0.529	1.828 / 1.832	**0.022 / 0.025**	**0.131 / 0.134**
	MLP	**0.098 / 0.099**	0.833 / 0.836	**0.092 / 0.092**	0.488 / 0.493	0.152 / 0.152	0.131 / 0.134
	SVR	0.139 / 0.139	**0.784 / 0.786**	0.109 / 0.111	**0.196 / 0.203**	0.146 / 0.146	0.345 / 0.345
5×5	Polynomial	0.180 / 0.189	1.084 / 1.092	0.231 / 0.232	0.817 / 0.822	**0.023 / 0.026**	**0.038 / 0.046**
	MLP	**0.088 / 0.093**	0.417 / 0.424	**0.161 / 0.162**	**0.398 / 0.401**	0.067 / 0.067	0.240 / 0.241
	SVR	0.154 / 0.157	**0.316 / 0.329**	0.174 / 0.175	0.509 / 0.515	0.029 / 0.032	0.170 / 0.176
8×8	Polynomial	0.073 / 0.074	**0.064 / 0.071**	**0.023 / 0.027**	0.210 / 0.212	0.076 / 0.077	0.158 / 0.161
	MLP	**0.066 / 0.067**	0.187 / 0.189	0.054 / 0.055	**0.036 / 0.053**	0.046 / 0.048	**0.093 / 0.101**
	SVR	0.086 / 0.088	0.143 / 0.151	0.095 / 0.097	0.256 / 0.264	**0.037 / 0.039**	0.195 / 0.198

- Refining calibration grid from 3×3 to 8×8 **reduces PMMA RMSE** by 10–30× across all methods
- MLP handles Al best on coarse grids, SVR recovers PMMA best at low dose and Polynomial Regression becomes competitive on denser grids.
- Higher dose alone cannot compensate for a coarse calibration grid — accuracy only improves when both photon statistics and grid density increase together **8×8 grid at 1.7–7.5 mAs is the optimal operating range, with MLP as the most robust single-model choice** (RMSE ≲ 0.2 cm)

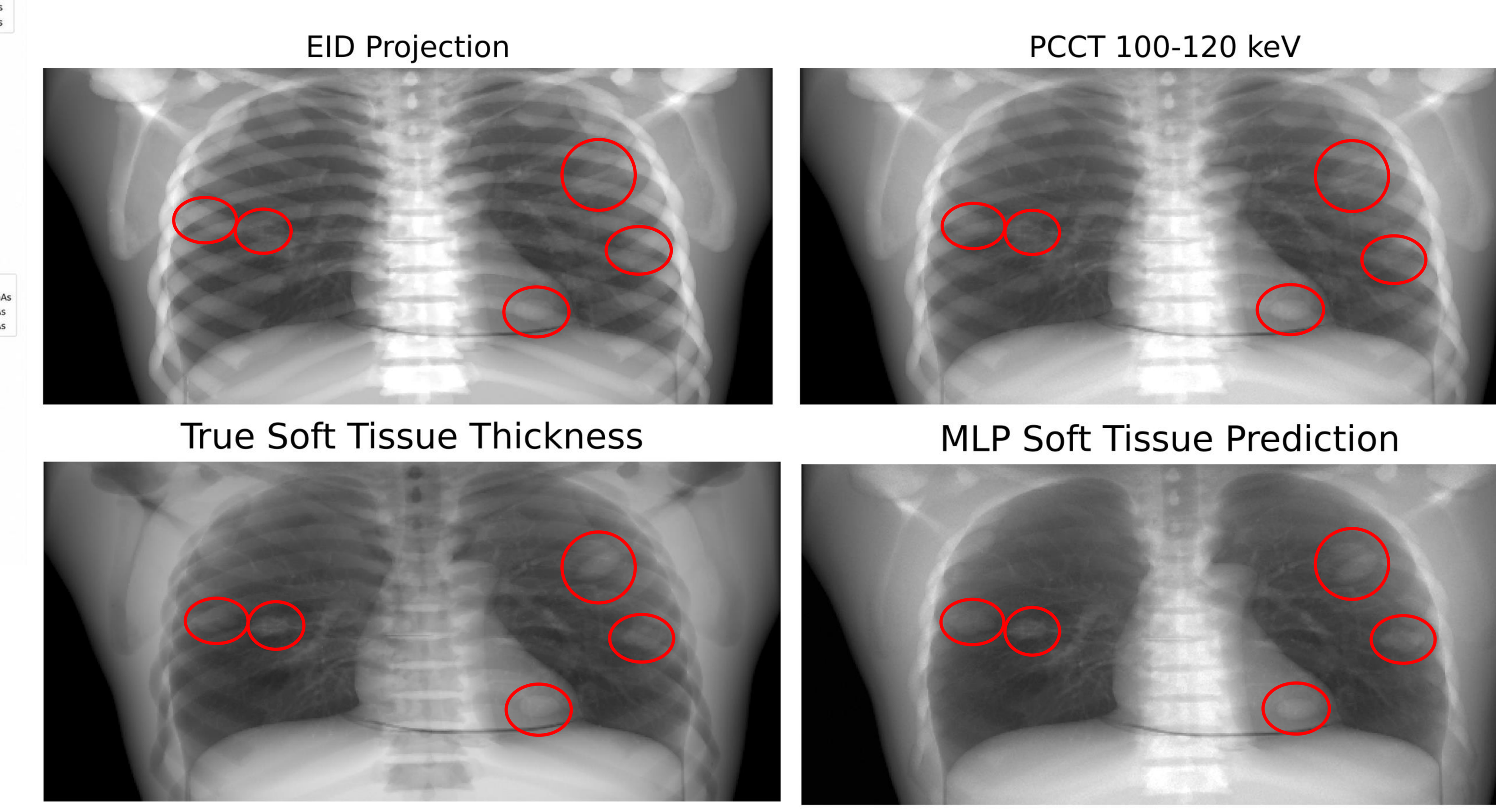
Contrast-to-Noise Ratio



Analysis of MLP CNR Performance

- PMMA shows **consistently higher CNR than aluminum** because its lower attenuation better matches soft tissue.
- Higher photon **dosage increases CNR** due **to improved photon counting statistics.**
- CNR generally **converges** as calibration grid size increases, with **the 8×8 grid showing greater stability**.
- Larger grids **reduce Poisson noise**, leading to more **reliable measurements**.

Synthetic Chest Phantom



Lung Nodule Detection

- Qualitative assessment of lung nodule visibility shows significant improvement to visibility of nodules hidden behind bone.
- Improved diagnostic capability and monitoring of potentially malignant nodule growth

References

Jeon, D., Lim, Y., Yang, H., Park, M., Kim, K., & Cho, H. (2025). Improving decomposition image quality in dual-energy chest radiography using two-dimensional crisscrossed anti-scatter grid. *Medical Physics*, *52*(7). https://doi.org/10.1002/mp.17819
Marupudi, S., & Ghammraoui, B. (n.d.). Comparative evaluation of machine learning and conventional material decomposition algorithms for spectral chest radiography using a CdTe photon-counting detector. U.S. Food and Drug Administration, Division of Imaging, Diagnostics, and Software Reliability
National Institute of Standards & Technology. (2009a, September 17). *NIST: X-Ray Mass Atten. Coef. - Polymethyl Methacrylate*. Physics.nist.gov. https://physics.nist.gov/PhysRefData/XrayMassCoef/ComTab/pmma.html
National Institute of Standards & Technology. (2009b, September 17). *XCOM: Photon Cross Sections Data for Aluminum*. Physics.nist.gov. https://physics.nist.gov/cgi-bin/Xcom/xcom3_1
Poludniowski, G., Omar, A., Bujila, R., & Andreo, P. (2021). Technical Note: SpekPy v2.0—a software toolkit for modeling x-ray tube spectra. *Medical Physics*, *48*(7). https://doi.org/10.1002/mp.14945
Zhao, B. (2015). Lung Phantom (Version 2) [Data set]. The Cancer Imaging Archive. https://doi.org/10.7937/k9/tcia.2015.08a1ixoo

Acknowledgements

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