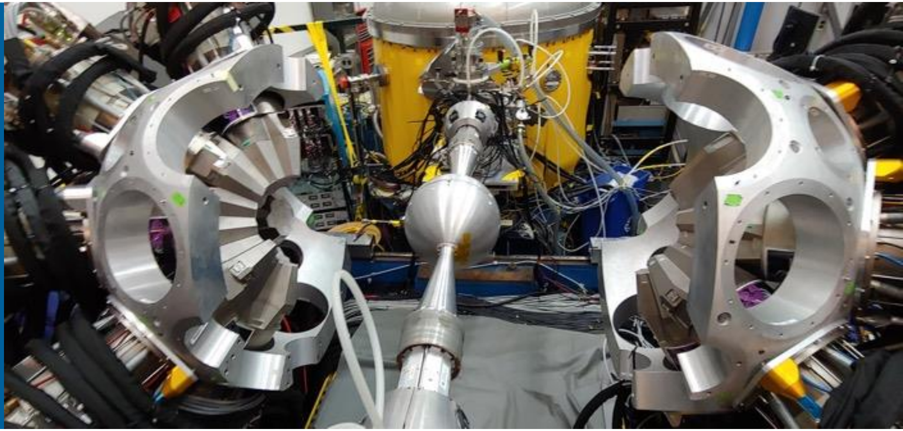
PRESENTATION TO NUCLEAR PHYSICS AI AND DATA SCIENCE, PI EXCHANGE MEETING

DEVELOPING MACHINE-LEARNING TOOLS FOR GAMMA-RAY ANALYSIS



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U.S. DEPARTMENT OF ENERGY
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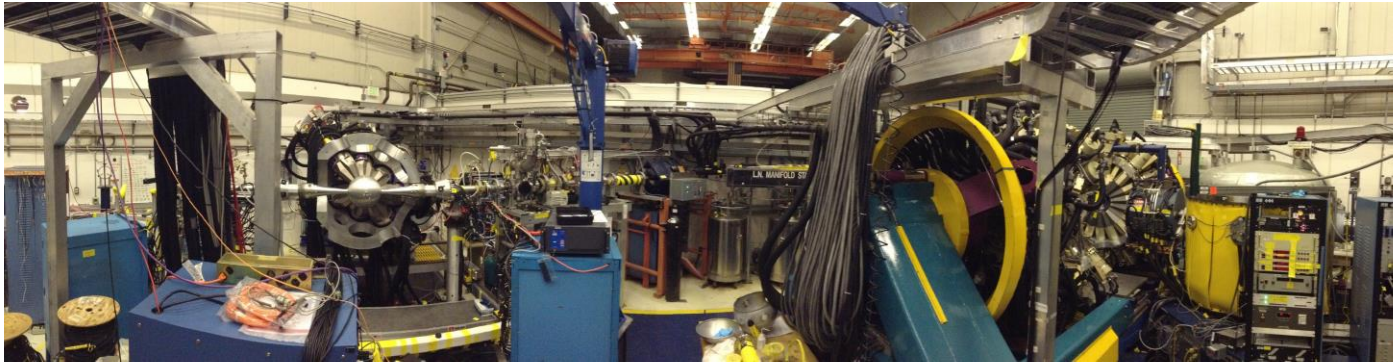
PROJECT PURPOSE AND GOALS

The **purpose** of this project is to develop automated decision-support tools to assist physicists in the analysis of complex experimental data taken with the large gamma-ray spectrometers (Gammasphere, GRETINA and AGATA).

Goals:

1. Develop machine-learning tools to improve γ-ray tracking (GRETINA/GRETA).
2. Develop machine-learning tools to assist in the construction of complicated level schemes using γ-γ and γ-γ-γ coincidence data.



PROJECT OUTLINE

Machine-Learning (ML) tools for Gamma-Ray Analysis

Gamma-ray Tracking

- Develop new methods to improve on current gamma-ray tracking algorithms to increase both photopeak efficiency and background rejection.
- Utilize machine learning tools to improve on these methods.
- Extend these methods to include pair production events.
- Incorporate these tools into tracking codes used by the community.

Thomas Lynn (ANL)

Level Scheme Construction

- Develop a mathematical toolkit to build levels schemes using both 2-fold and 3-fold coincidence information bench marking with known level schemes.
- Develop tools to automatically extract intensity information from gamma-ray coincidence data (2D, 3D).
- Apply toolkit to both simulated data and experimental data taken with Gammasphere and GRETINA.

Tamas Budner/David Lenz (ANL)

PROJECT PARTICIPANTS

Joint project between two ANL divisions: Physics (PHY) and Math and Computer Science (MCS)

PHY

- Tamas Budner (FOA funded Pdoc)*
- Mike Carpenter (ANL Staff)*
- Filip Kondev (ANL Staff)
- Amel Korichi (IJCLab Orsay Staff)**
- Torben Lauritsen (ANL Staff)
- Marco Siciliano (ANL Staff)

MCS

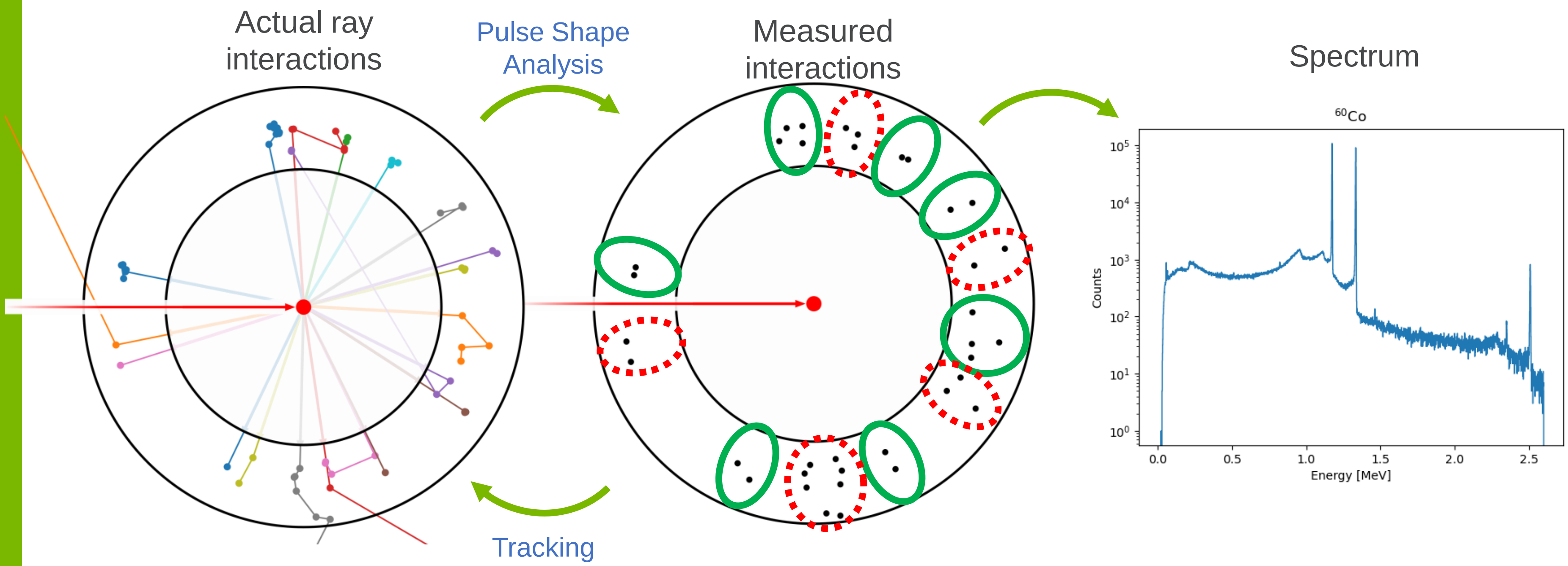
- David Lenz (ANL Staff, 25% FOA)*
- Sven Leyffer (ANL Staff)
- Thomas Lynn (FOA funded Pdoc)*
- Robert Ross (ANL Staff)

* Today's Presenters

** On Sabbatical at ANL starting January 2023

ML TOOLS FOR GAMMA-RAY TRACKING

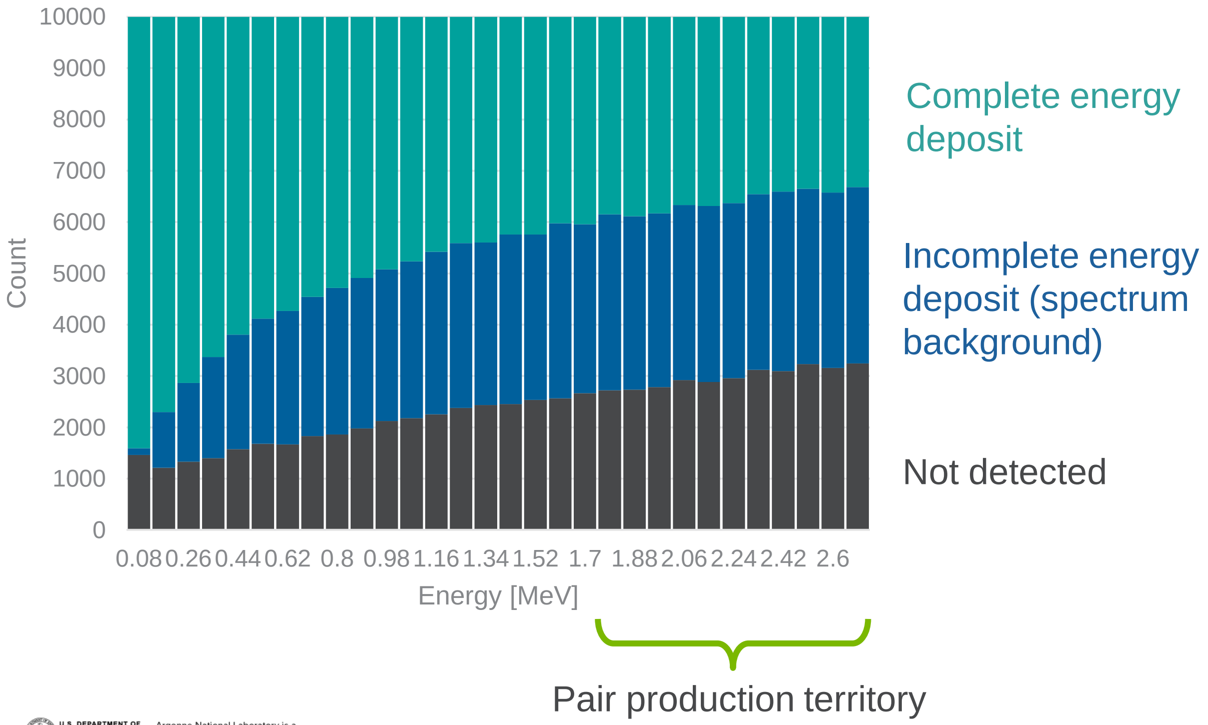
GAMMA-RAY TRACKING



Tracking: *Cluster* the measured interactions and put them in *order* replicate actual event

Suppression: Remove poor quality “rays” from gamma spectrum

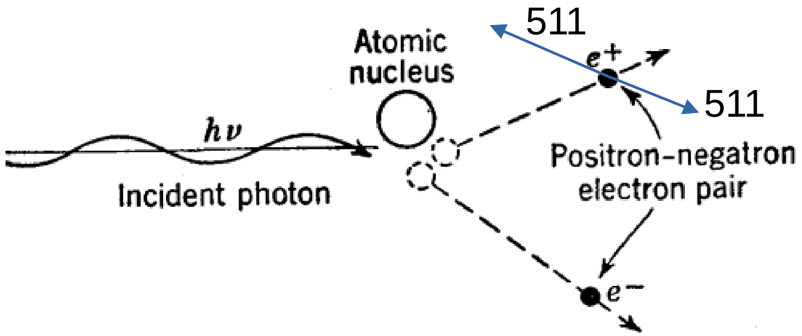
WHERE ARE GAMMA-RAYS LOST?



Other losses:

- Clustering interactions
  - Bad clusters move peak data to background
- Ordering interactions
  - Bad orders move peak data (Doppler) to background
- Suppressing gamma-rays
  - Bad suppression removes peak data over background

PAIR PRODUCTION EVENTS



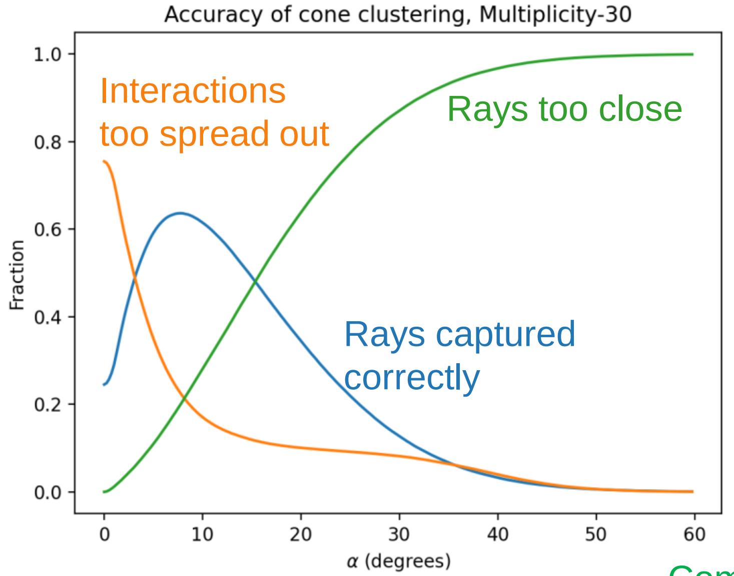
$$h\nu = (T_- + m_0c^2) + (T_+ + m_0c^2)$$

- Look for the flash of kinetic energy of the e^+ and e^- $(T_- + T_+)$
- Then look for 2×511 keV gamma-rays, or one 1022 keV gamma-ray, nearby (centimeters)
- Note: the 511's should not be Doppler corrected as they are emitted at rest
- The first interaction is taken to be the barycenter of the flash points
- The sharing of the e^+/e^- kinetic energy is near random
- Flash energy is in general several MeV, thus, distinguishable from Compton scattering

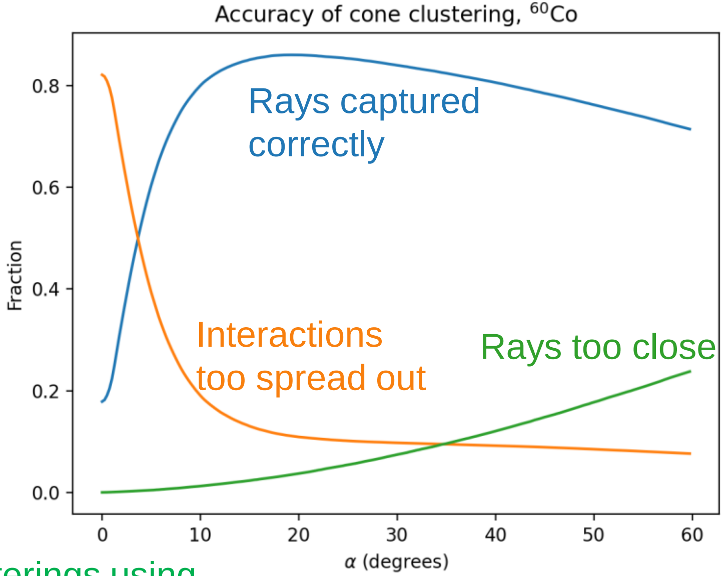
GEOMETRIC (CONE) CLUSTERING

How often are the interactions clustered correctly into a gamma-ray?

High multiplicity: Accuracy is limited (maximum ~60% of gamma-rays recovered)



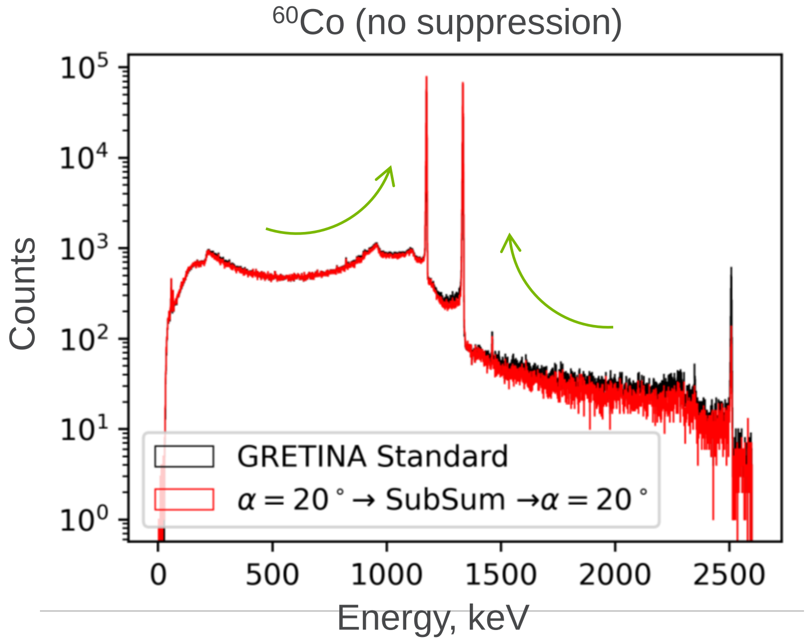
Low multiplicity: Accuracy often very high (>80% of gamma-rays recovered)



Comparing clusterings using ML is continuing work

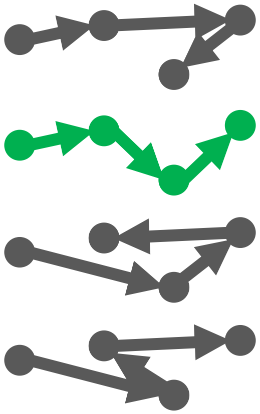
ENERGY SUM CLUSTERING

- Cluster using interaction energies to find gamma-rays with specific energies
  - Subset-Sum method
- Useful for:
  - *Pair production (511 keV rays) (Continuing work)*
  - Low multiplicity data
  - Known level scheme data
- Difficulties:
  - Doppler correction changes energies
  - Creates false peak counts



OPTIMIZING INTERACTION ORDER FOR DOPPLER CORRECTION

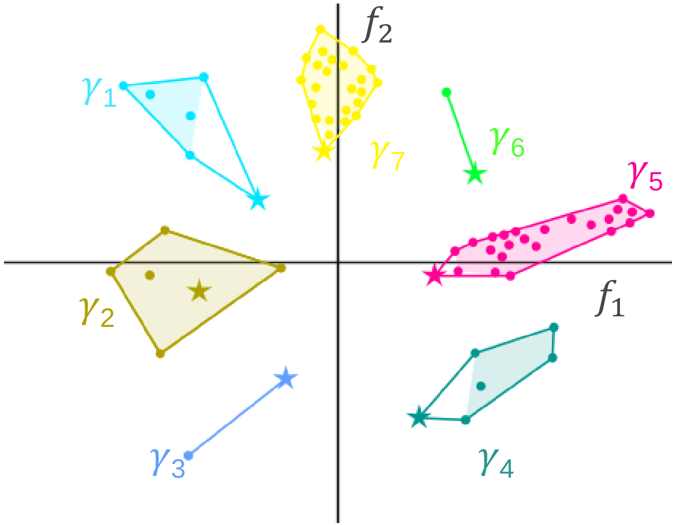
- Interaction order is needed for Doppler correction
  - Common with high v/c data that will be produced at FRIB
- Chosen by Figure-Of-Merit (FOM) value



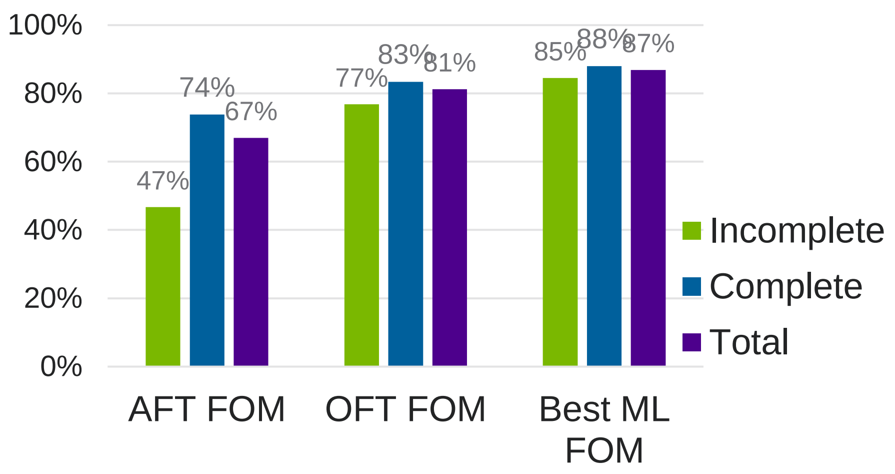
	Gamma-ray interaction order	FOM_1	FOM_2	$FOM_1 + FOM_2$
a)		$\boxed{1}$	3	2
b)		2	2	$\boxed{1}$
c)		4	4	4
d)		3	$\boxed{1}$	3

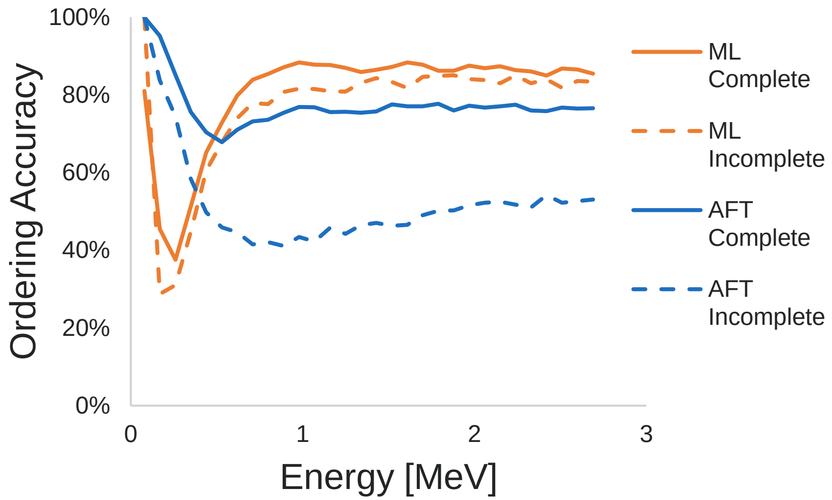
Formally a *Learning-to-rank (LTR)* problem (e.g., search engine optimization)

Combination of FOMs and other features are used to directly optimize an ordering objective



ACCURACY OF ORDERING FOM: MULTIPLICITY-30 DATA





LTR increases ordering accuracy for all gamma-rays by 6-7%

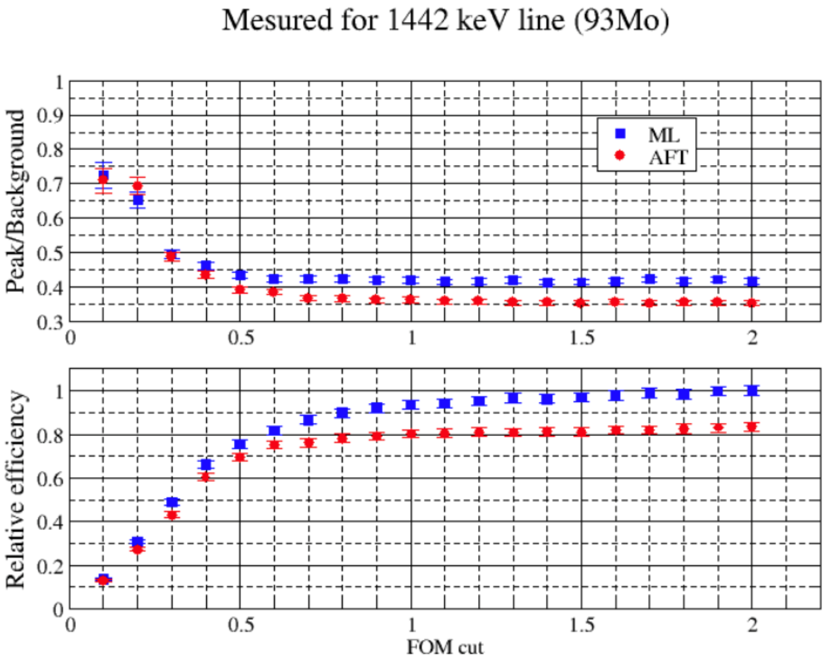
Features/FOMs used by LTR are computationally expensive (Computational speed, continuing work)

Accuracy is energy dependent

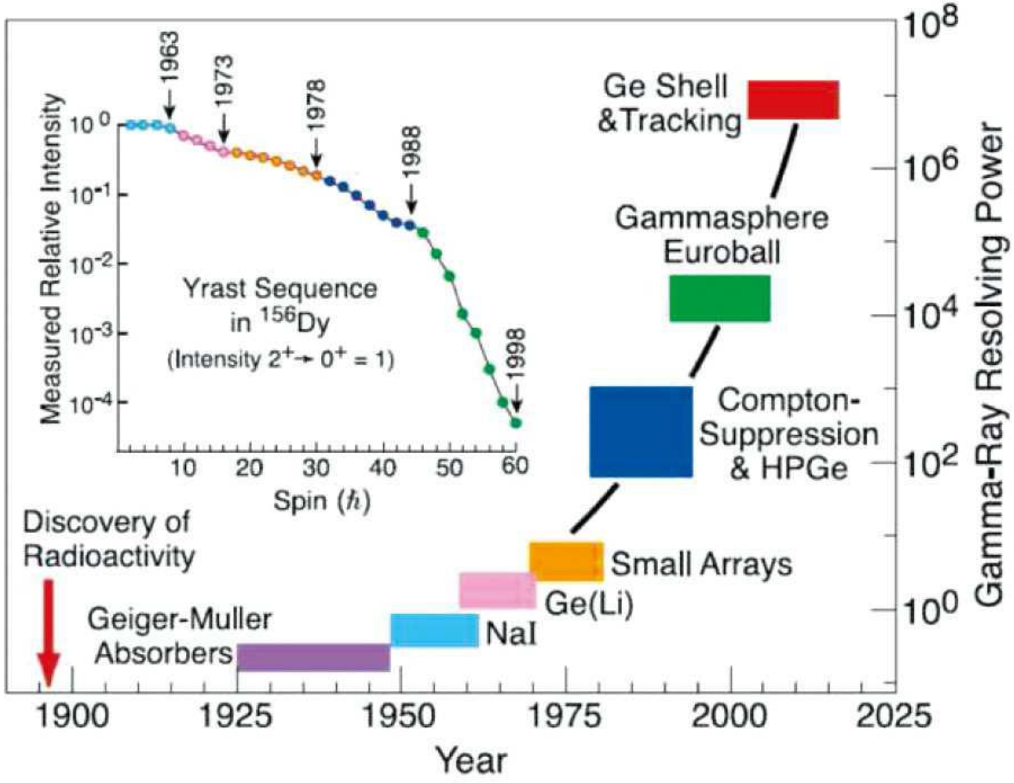
Energy specific models may be valuable (Continuing work)

ORDERING ACCURACY LEADS TO DOPPLER CORRECTION IMPROVEMENT

- For high v/c, ~8% improvement in peak sharpening
  - Better resolving power
  - Less background counts
  - More peak counts
- Important for FRIB measurements
- For FOM > 0.5:
  - 10-15% improved Peak/Background
  - 9-12% improved efficiency
- Small improvements greatly effect the resolving power of the detector



ORDERING ACCURACY IMPROVES RESOLVING POWER OF GRETINA/GRETA



$$r \approx \left(\frac{SE}{\delta E}\right)\left(\frac{P}{T}\right)$$

SE: average energy spacing
δE: "effective E-resolution" (ΔE_{det} and $\Delta E_{\mathrm{Doppler}}$)

Resolving Power $= r^{\mathrm{Fold}}$

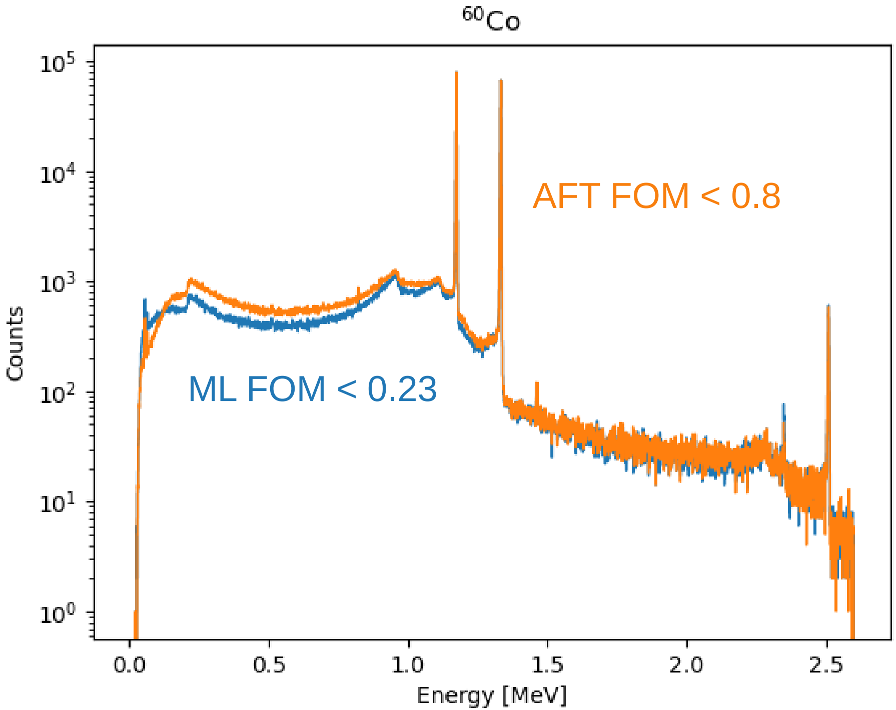
For a 5-fold gamma-ray event:

- 10% increase in P/T → ~60% increase in resolving power
- 8% improvement in δE → ~50% increase in resolving power
- Both → ~140% increase in resolving power

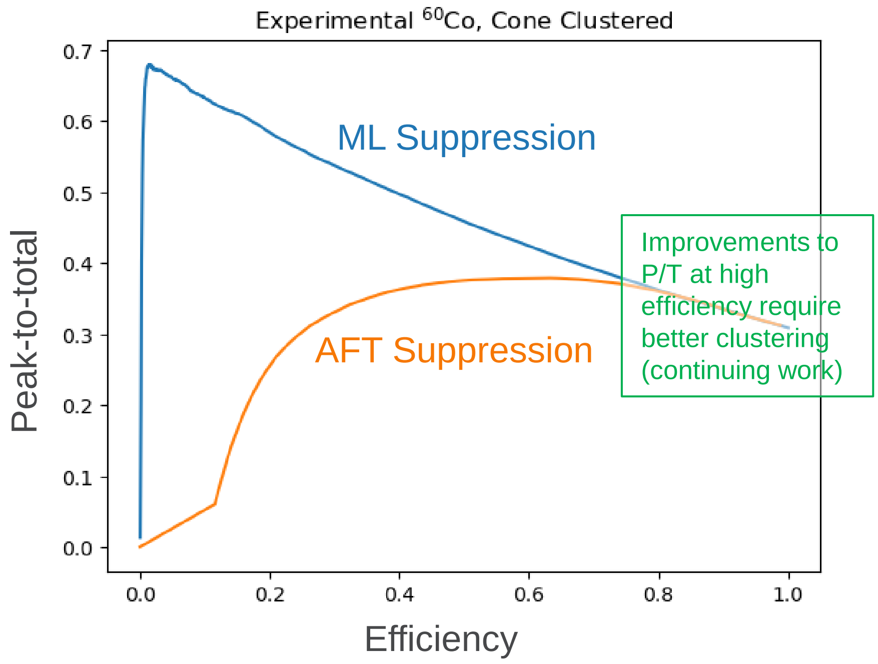
SUPPRESSION USING NEW FEATURES

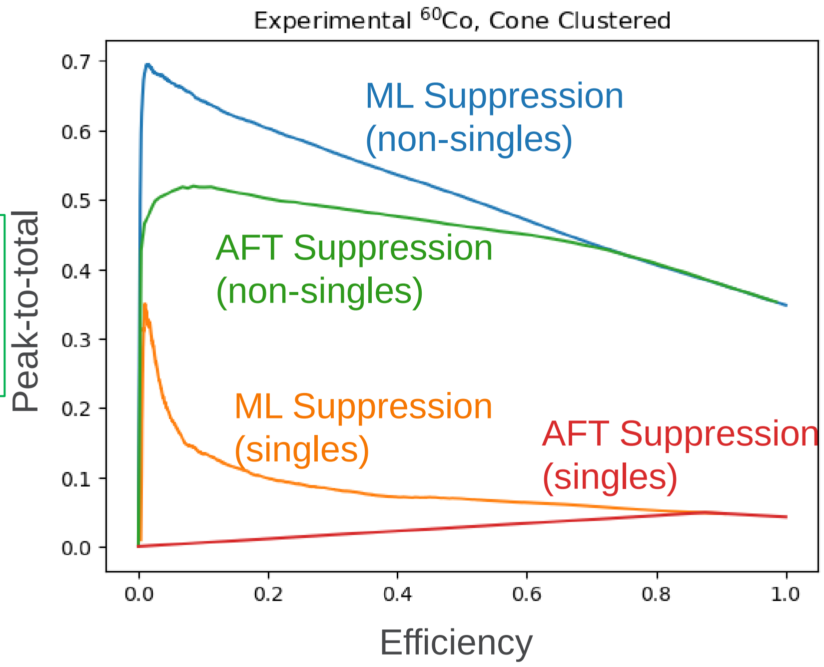
- Features created for LTR ordering can be used for determining which rays to remove from the final spectrum
- Suppression is improved overall
- *Accuracy depends on energy*

New features improve suppression with little change in computational cost



SUPPRESSION USING NEW FEATURES: EXPERIMENTAL ^{60}CO



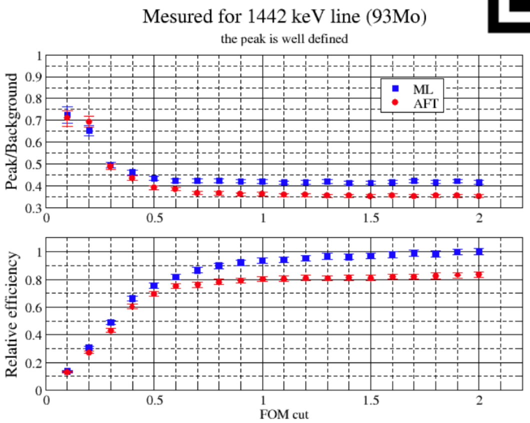


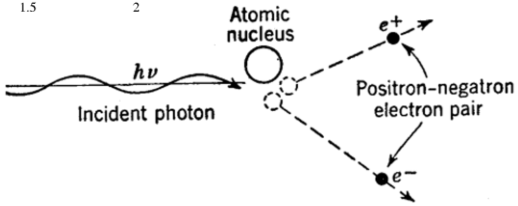
Suppression FOM transfers some performance to experimental data
(Energy specific models are continuing work)

github.com/lynntf/GRETO

GAMMA-RAY TRACKING PROGRESS

- Current project milestones, (nearly complete)
  - Python Code published on GitHub
  - New ordering approaches improve upon existing methods up to 2.4× in resolving power for Doppler corrected data
  - LTR methods expand possible tracking optimizations
  - Journal paper manuscript in preparation
- Renewal project milestones (continuing)
  - New suppression approaches further improve resolving power and transfer to experiments (nearly complete)
  - Pair production tracking for higher energy (>7 MeV) gamma-rays

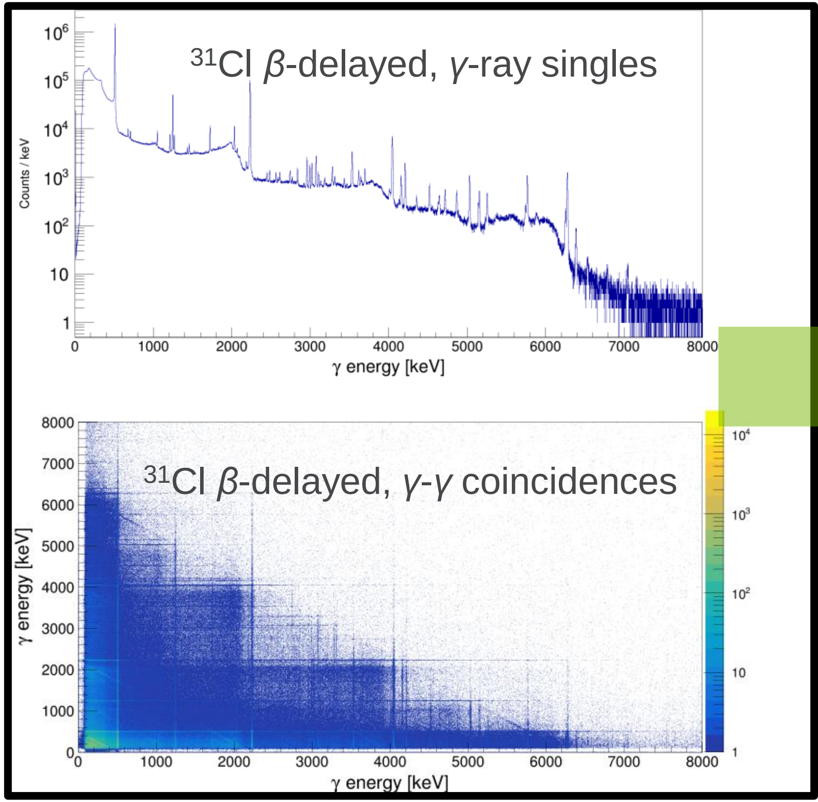




ML TOOLS FOR LEVEL-SCHEME DESIGN

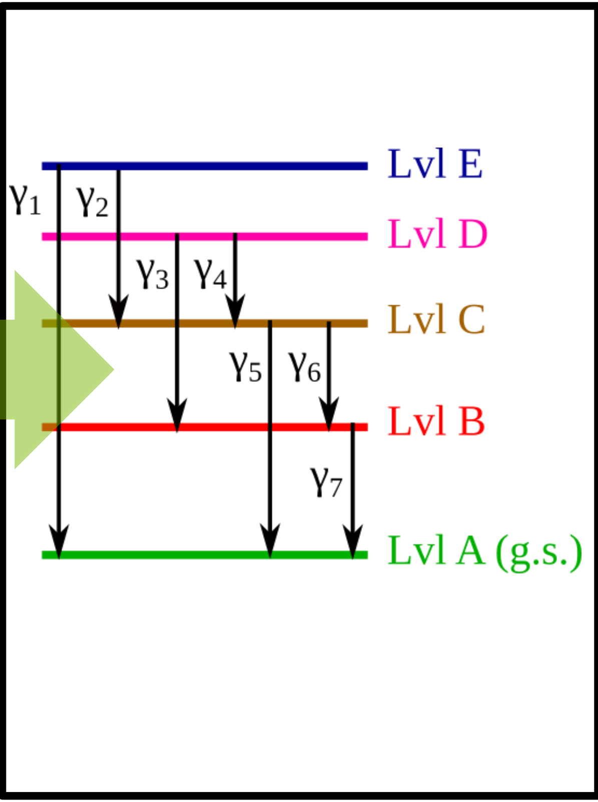
NUCLEAR LEVEL SCHEME CONSTRUCTION

Numerically solving decay scheme from gamma-ray data



$$S = \begin{pmatrix} S_1 \\ S_2 \\ \cdots \\ S_n \end{pmatrix}$$

$$C = \begin{pmatrix} 0 & C_{i,j} & \cdots & C_{i,j} \\ C_{i,j} & 0 & & \vdots \\ & & 0 & \\ \vdots & & & \ddots \\ C_{i,j} & \cdots & & 0 \end{pmatrix}$$



NUCLEAR LEVEL SCHEME CONSTRUCTION

Automating analysis steps

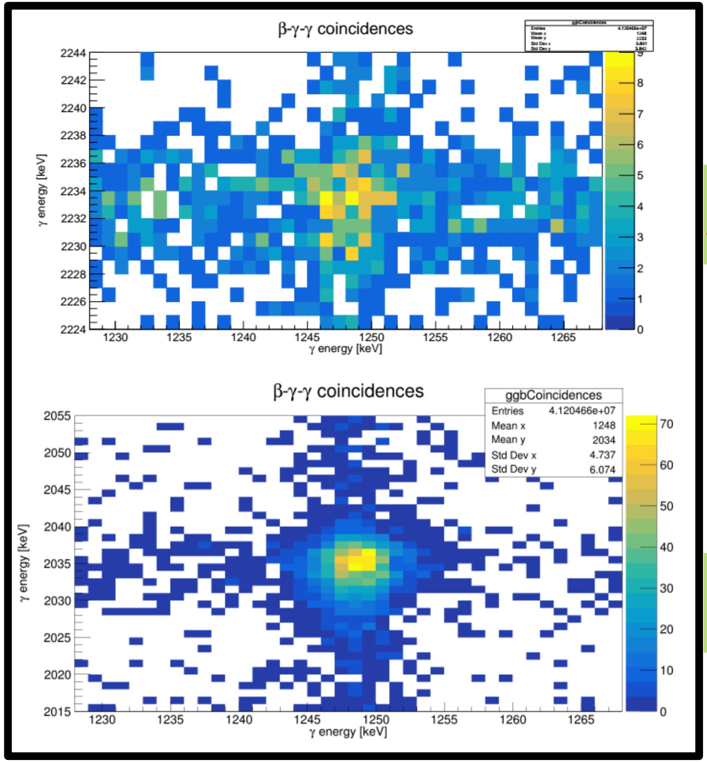
1. Extract γ-ray transition intensities S and γ−γ coincidences C
   - Background subtraction
   - Fit photopeaks 1D γ-ray singles spectrum
   - Fit 2D γ−γ coincidences spectrum
2. Numerically solve inverse optimization problem in matrix representation
   - Demonstrate proof of principle
   - Benchmarking performance
   - Apply constraints to improve accuracy and efficiency
3. Construct nuclear decay scheme from adjacency matrix A
   - Create transition-centric graphic
   - Mapping from transition space to level-centric space
   - Assign excitation energies and other nuclear properties
   - Plot and compare to literature

NUCLEAR LEVEL SCHEME CONSTRUCTION

Step 1: Extract γ-ray transition intensities *S* and γ–γ coincidences *C*

- Multidimensional background subtraction

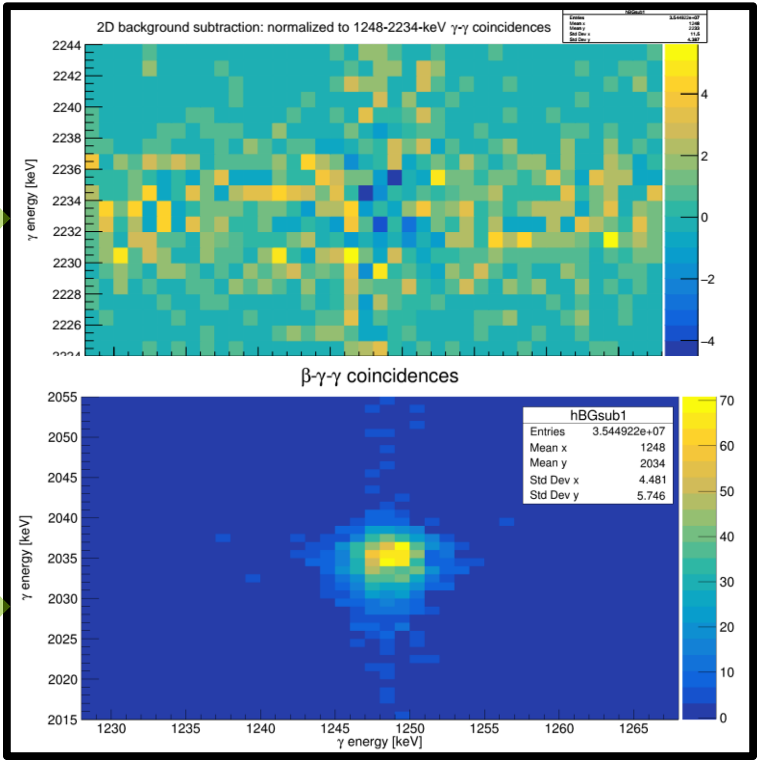
Before



Accidental

True

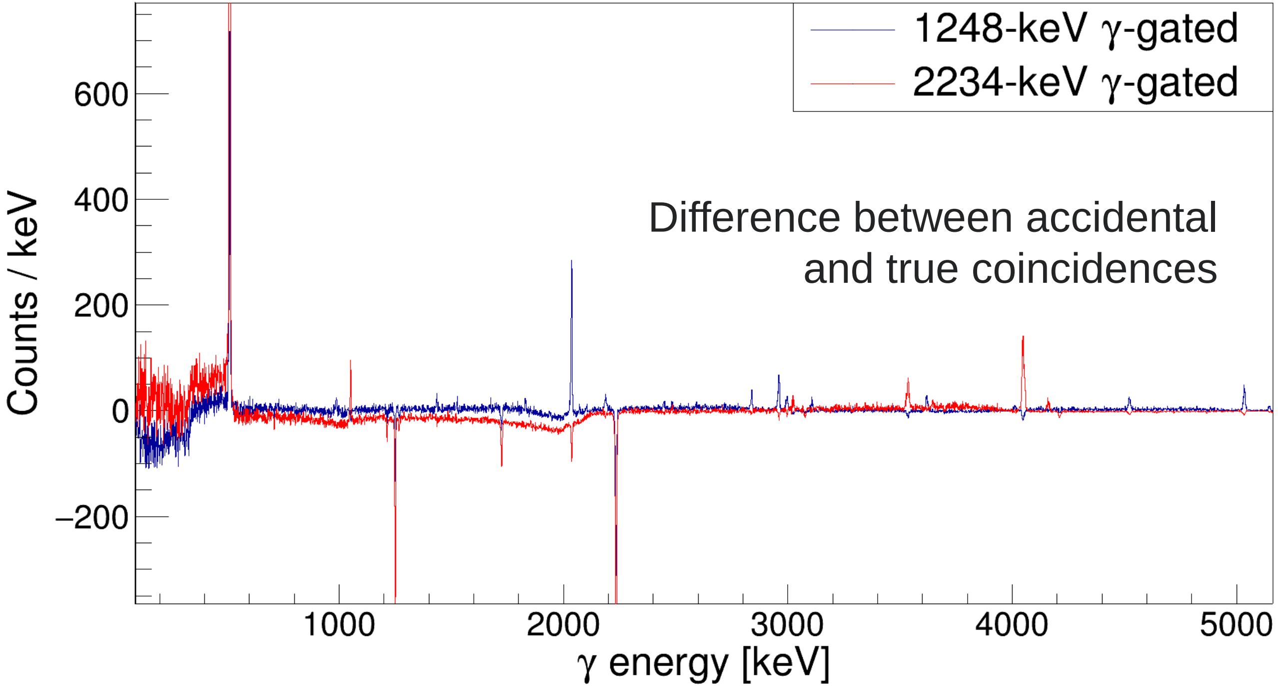
After subtraction



NUCLEAR LEVEL SCHEME CONSTRUCTION

Step 1: Extract γ-ray transition intensities *S* and γ–γ coincidences *C*

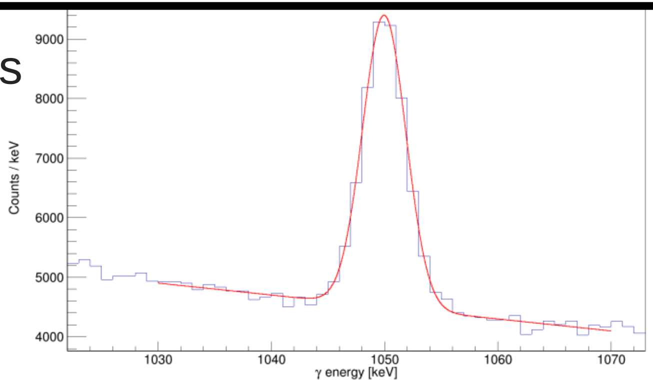
- Projecting on coincidence cuts
- Peak identification and fitting



NUCLEAR LEVEL SCHEME CONSTRUCTION

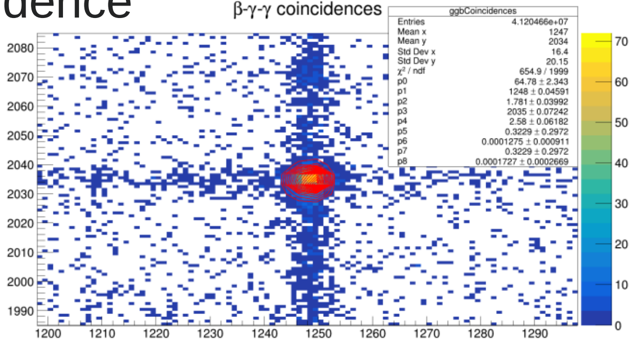
Step 1: Extract γ-ray transition intensities *S* and γ–γ coincidences *C*

Fit 1D singles spectrum



$$S = \begin{pmatrix} S_1 \\ S_2 \\ \cdots \\ S_n \end{pmatrix}$$

Fit 2D coincidence spectrum



$$C = \begin{pmatrix} 0 & C_{i,j} & \cdots & C_{i,j} \\ C_{i,j} & 0 & & \vdots \\ & & 0 & \\ \vdots & & & \ddots \\ C_{i,j} & \cdots & & 0 \end{pmatrix}$$

MATHEMATICAL FORMULATION

Writing Level Scheme Construction as Matrix Equations

- Start with data from Gamma-Sphere experiment:
  - S: γ-ray transitions & intensities (as diagonal matrix)
  - C: γ-γ coincidence data
- Determine the outputs:
  - A: the matrix of branching ratios
  - D: the directed coincidence data
- Following Demand (2013), we try to satisfy two equations simultaneously:

$$D = S\left((I - A)^{-1} - I \right) \quad \text{and} \quad C = D + D^T$$

NUCLEAR LEVEL SCHEME CONSTRUCTION

Step 2: Numerically solve inverse optimization problem in matrix representation

- We have two governing equations:

$$D = S((I - A)^{-1} - I)$$
$$C = D + D^T$$

- Satisfying both equations leads to the nonlinear optimization problem:

$$\min_{A,D} \left\| D - S\left((I - A)^{-1} - I\right) \right\|^2$$

$$\text{subject to: } A \geq 0, \sum_j A_{ij} \leq 1, C = D + D^T$$

Finding A, D that produce the global minimum value is equivalent to finding A, D that satisfy the governing equations (and thus describe the true level scheme)

IMPROVEMENTS IN OPTIMIZATION

Not all Optimization Problems Created Equal

Element-wise multiplication

$$\min_{A,D} \left\| D - S\left((I-A)^{-1} - I\right) \right\|^2$$
subject to:
$$A \geq 0,$$
$$\sum_j A_{ij} \leq 1,$$
$$C = D + D^T$$

$$\min_{A,D} \| D - ST \|^2$$
subject to:
$$A \geq 0,$$
$$\sum_j A_{ij} \leq 1,$$
$$C = D + D^T$$
$$(I - A)(T + I) = I$$

$$\min_{X,A} \| (X \circ C)A + SA - (X \circ C) \|^2$$
subject to:
$$A \geq 0,$$
$$\sum_j A_{ij} \leq 1,$$
$$X_{ij} + X_{ji} = 1$$

⇩ Calculating the inverse is far too computationally expensive

⇩ Optimization rarely converges, search space is highly non-convex due to new constraint

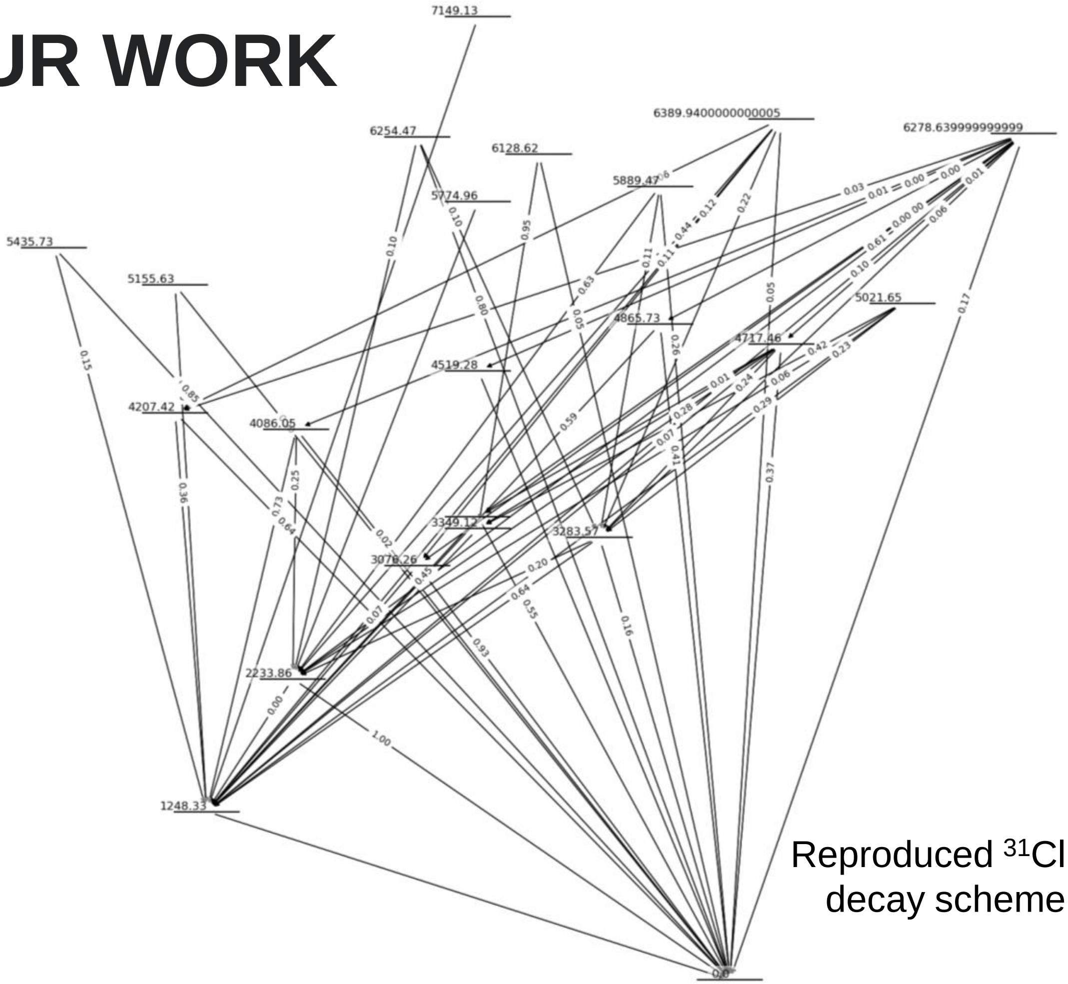
⇧ Better! Still, optimization may fail to converge at times

Restructuring the mathematical optimization into an equivalent form drastically improves efficiency and reliability

BENCHMARKING OUR WORK

Successful Outcomes

- Using Interior Point Optimizer (Ipopt) to solve large-scale, nonlinear optimization problem
- Creates perfectly consistent decay scheme within 2 - 20 minutes (running on a laptop) for schemes with up to ~80 transitions



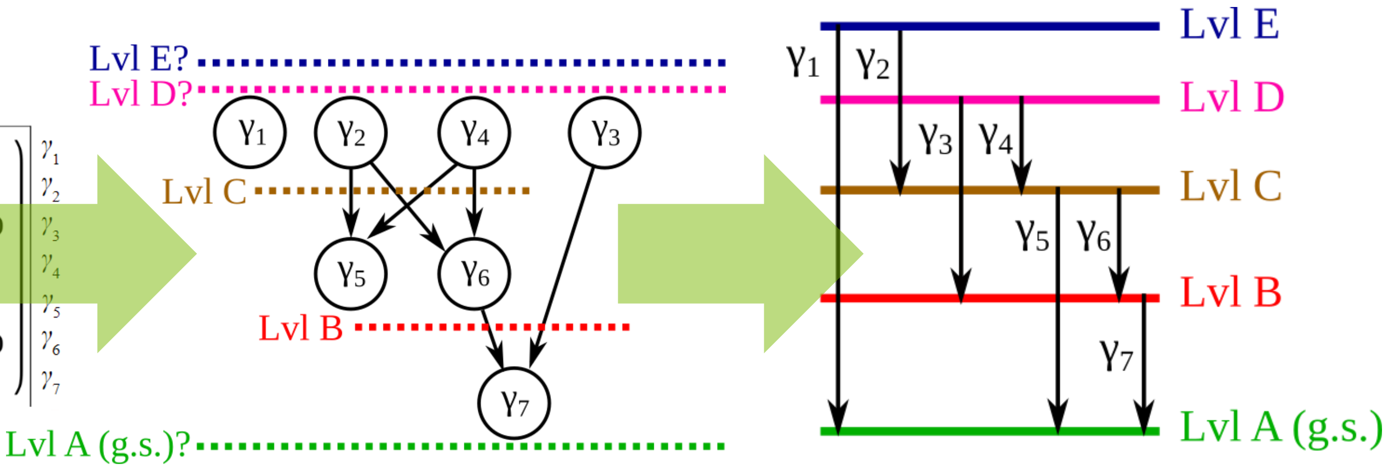
Reproduced ^{31}Cl decay scheme

NUCLEAR LEVEL SCHEME CONSTRUCTION

Step 3: Construct nuclear decay scheme from adjacency matrix *A*

- Create transition-centric graphic
- Mapping from transition space to level-centric space
- Assign excitation energies and other nuclear properties
- Plot and compare to literature

$$A = \begin{array}{c} \begin{array}{ccccccc} \gamma_1 & \gamma_2 & \gamma_3 & \gamma_4 & \gamma_5 & \gamma_6 & \gamma_7 \end{array} \\ \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.4 & 0.6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.0 \\ 0 & 0 & 0 & 0 & 0.4 & 0.6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \end{array} \begin{array}{c} \gamma_1 \\ \gamma_2 \\ \gamma_3 \\ \gamma_4 \\ \gamma_5 \\ \gamma_6 \\ \gamma_7 \end{array}$$



FUTURE WORK

Extending to Higher Dimensions

- *N*-fold coincidence data of *K* gamma-ray energies collected in *N*-dimensional tensor *T*:

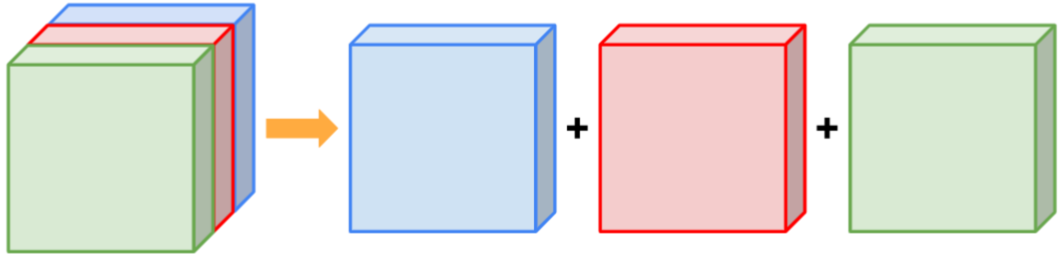
$$T \in \mathbb{R}^{\overbrace{K \times K \times \cdots \times K}^{N \text{ times}}},$$

- Can obtain matrix *M* that represents higher order coincidences by contracting the tensor *T* by summing over *N* – 2 dimensions:

$$M_{i,j} := \sum_{N} \sum_{i_3, i_4, \ldots, i_N} \left(T^{(N)}_{i,j,i_3,i_4,\ldots,i_N} \right), \quad \forall i, j = 1, \ldots, K.$$

- Solve the optimization problem:

$$\min_{A,D} \sum_{l=1}^{N(N-1)} \| D_l - S((I - A)^{-1} - I) \|^2 \quad \text{s.t. } C + \sum_{N} M_l^{(N)} = D_l + D_l^{\top}, \ \sum_j A_{i,j} \le 1, \ A \ge 0,$$



PLANNED ADDITIONAL WORK:

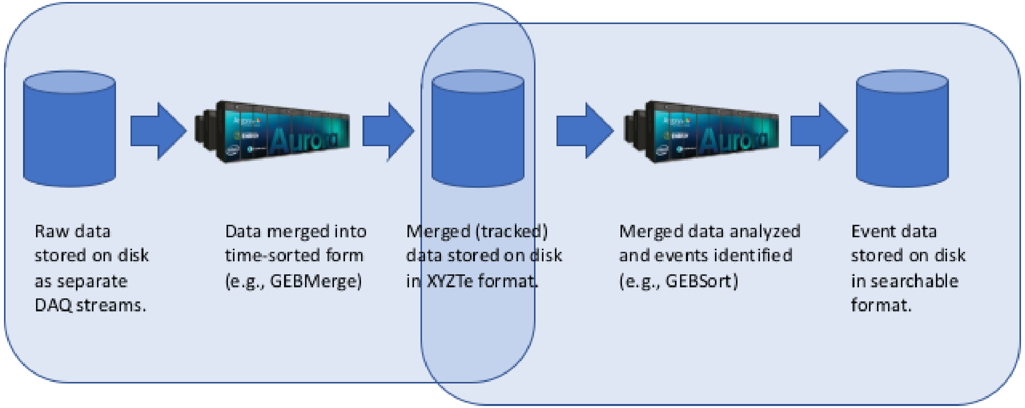
- DEVELOPING HPC ANALYSIS TOOLS

- IMPROVING COULOMB-EXCITATION ANALYSIS

DEVELOPING HPC ANALYSIS TOOLS

Goal: Accelerate workflow for γ-ray analysis via HPC and database technique

- Accelerate merge step on HPC
  - Perform parallel merge
  - Develop MPI for GRETINA
- Store data for fast query
  - Prepare for multi-fold analys
  - Leverage levelDB for storing data suitable for parallel search … accelerate γ-γ-γ coincidence extraction



IMPROVING COULOMB-EXCITATION ANALYSIS

Goal: Extending analysis to Coulomb-excitation experiments to extract precise information on structure of nuclear species

- Leverage open-source code GOSIA to minimize difference between computed and experimental yield:

$$\min_{M} \chi^2(M) := \underbrace{\frac{1}{N}\sum_{I} w_I \sum_{k\in I}\left(C_I Y_k^c(M) - Y_k^e\right)^2/\sigma_k^2}_{\text{Coulomb } \gamma-\text{yields}, S_y} + \underbrace{\sum_{j}\left(\frac{Y_j^c(M)}{Y_j^n} - u_j\right)_+^2/u_j^2}_{\text{observation limits}, S_1} + \underbrace{\sum_{i}\frac{d_i(M) - d_i^e}{\sigma_i^2}}_{\text{auxiliary terms}, S_a}$$

- Apply modern optimization and ML tools to solve χ^2 minimization (Newton solver for faster convergence)
- Reinforcement learning techniques in outer loop to learn matrix signs in *M*

BUDGET TABLE AND
TABLE OF DELIVERABLES AND SCHEDULE

BUDGET TABLE

Summary of expenditures by fiscal year (FY):

	FY21 ($k)	FY22 ($k)	Total ($k)
a) Funds allocated	500	500	1000
b) Actual costs to date	180 (FY22)	513 (FY23)	693

We have ~$307k remaining at the end of FY23. These remaining funds resulted in the fact that two full-time post-doctoral appointees paid from this project did not begin their appointments until later than FY22-Q1. Specifically, Dr. Thomas Lynn began his term in June 2022 and Dr. Tamas Budner began his term in October 2022. The remaining $307k covers the cost for Dr Lynn up to July 1, 2024, and Dr. Budner up to October 1, 2024 which would mark two years of support from the current project for both individuals. These funds are being rolled over into our renewal grant.

MAJOR DELIVERABLES AND SCHEDULE

ML Tools for Gamma-Ray Tracing and Level-Scheme Construction

Area	Project	Deliverable	Timeline
γ-Ray-Tracking	ML for Tracking	Python code	Dec 23
Level-Scheme (2D)	Inverse Optimal Design	Python code	May 23
γ-Ray-Tracking	ML for Tracking	Journal paper	Feb 24
Level-Scheme (2D)	Optimal Level-Scheme	Journal paper	Apr 24
γ-Ray-Tracking	Pair Production	Python code	Oct 24
Level-Scheme (3D)	ML Solver & Construction	Python code	Oct 24

MODERN ML & OPTIMIZATION TOOLS FOR TRACKING AND LEVEL-SCHEME DESIGN