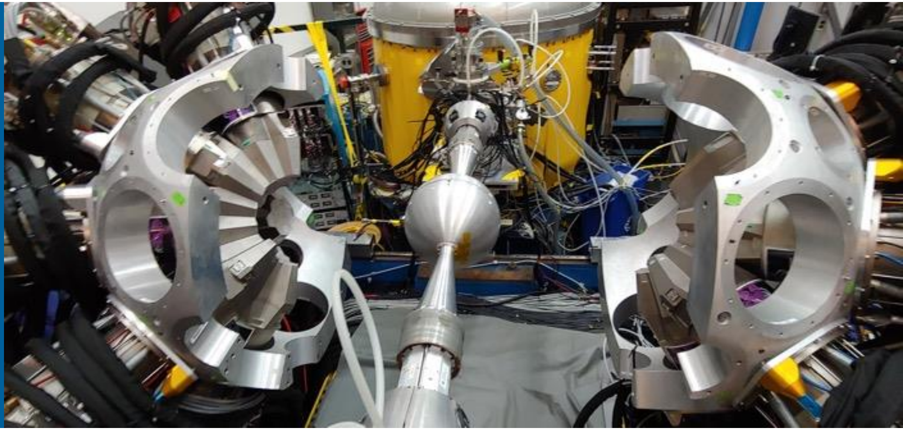
PRESENTATION TO NUCLEAR PHYSICS AI AND DATA SCIENCE, PI EXCHANGE MEETING

DEVELOPING MACHINE-LEARNING TOOLS FOR GAMMA-RAY ANALYSIS



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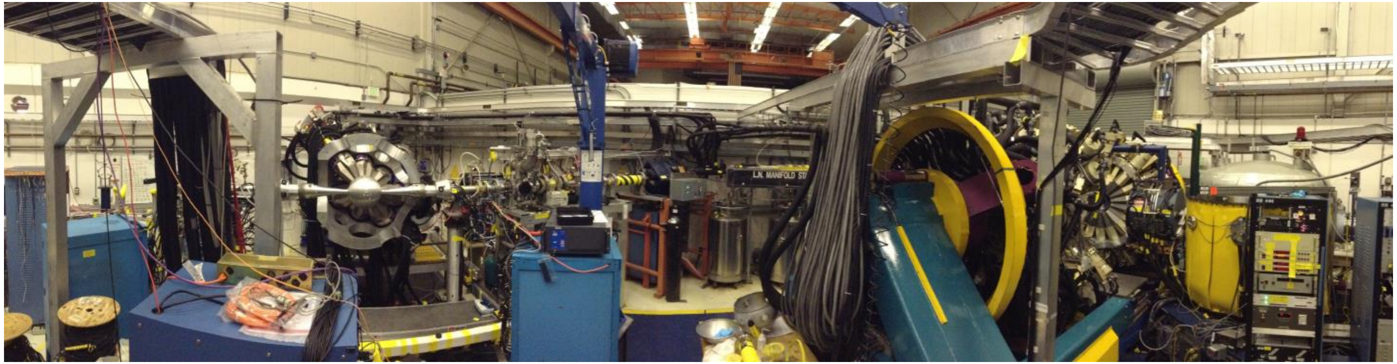
PHASE I: PROJECT PURPOSE AND GOALS

The **purpose** of phase I 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.



PHASE I/II - 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.

T. Lynn, T. Lauritsen, A. Korichi (ANL)

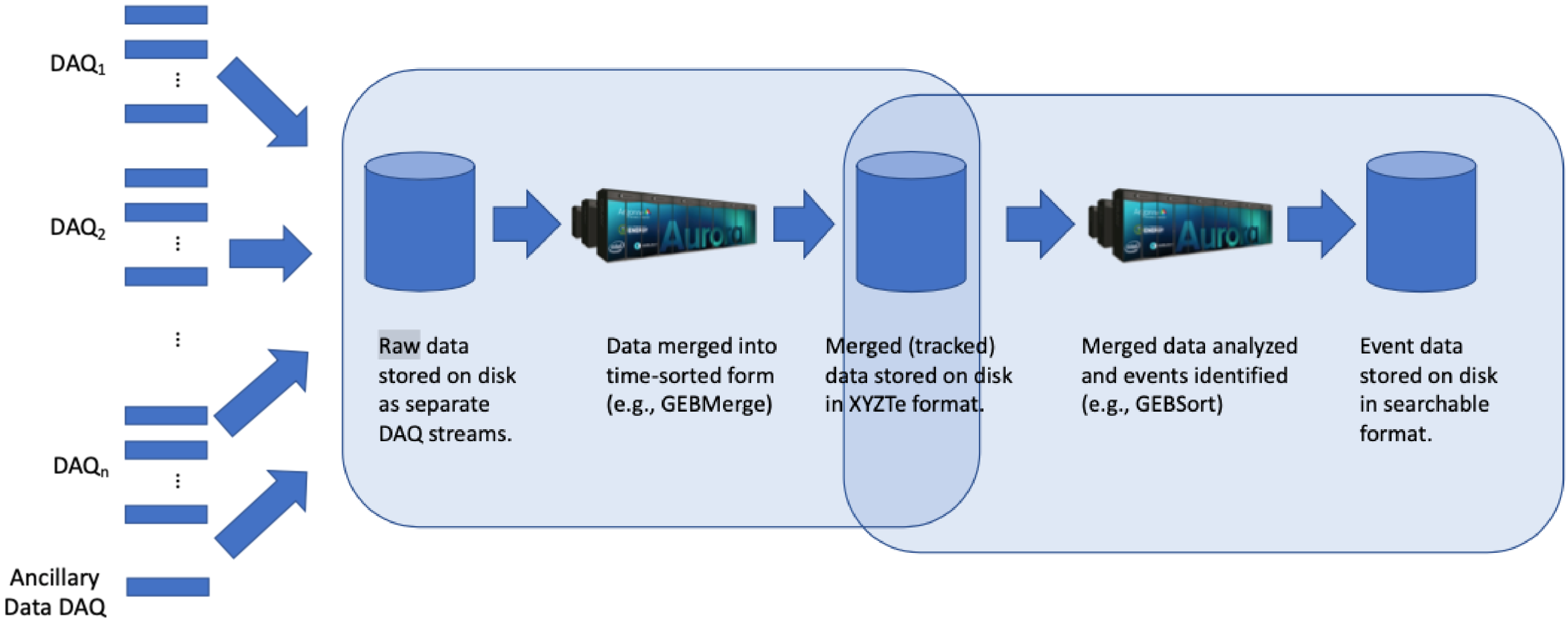
Level Scheme Construction

- 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.

T. Budner, D. Lenz, M. Carpenter

PHASE II - ADDITIONS

HPC Tools for Gamma-Ray Analysis



PHASE II - ADDITIONS

Optimization and ML tools for Coulomb excitation

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

We are investigating the use of modern machine-learning and optimization techniques to accelerate the least-squares optimization in GOSIA. Our developments will enable other outer loop analysis, such as the automatic selection of weights and the use of reinforcement learning techniques for the determination of matrix signs. (Leyfer and Siciliano)

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)
- Sven Leyffer (ANL Staff)
- Thomas Lynn (FOA funded Pdoc)
- Robert Ross (ANL Staff)
- Rob Latham (ANL Staff)

** Today's Presenters

BUDGET TABLE

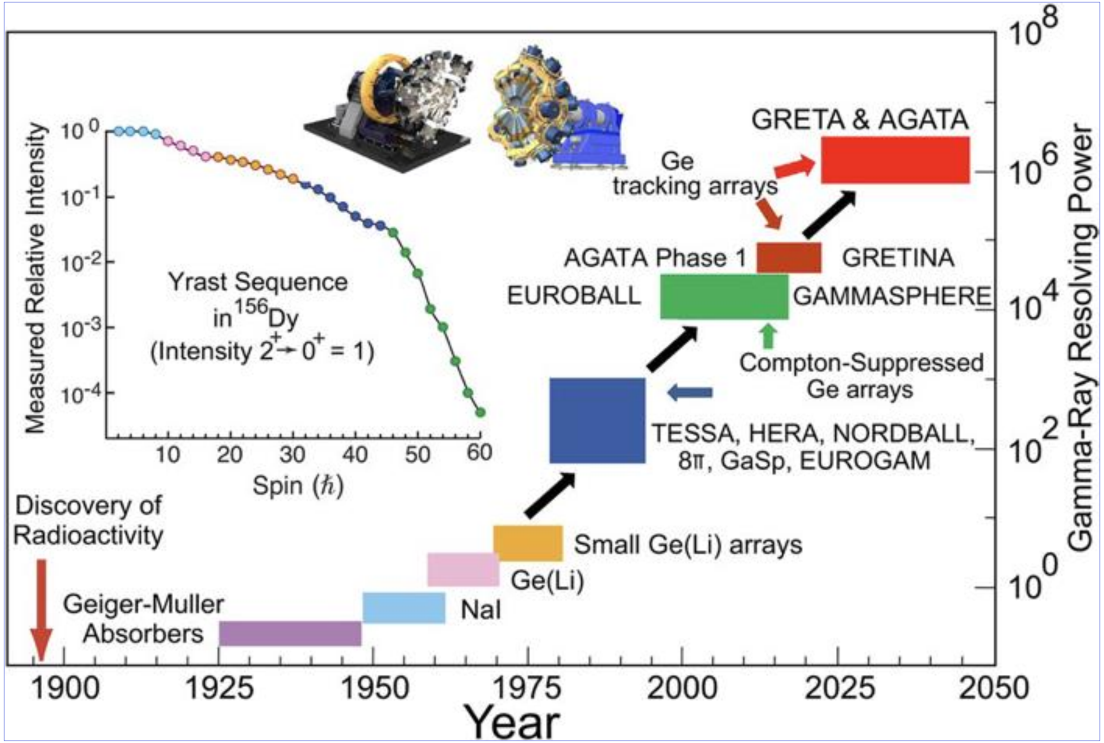
Summary of expenditures by fiscal year (FY):

	FY21 ($k)	FY22 ($k)	FY23 ($k)	FY24 ($k)	Total ($k)
a) Funds allocated	500	500	0	820	1,820
b) Costs to date	0	179	392	435	1,006

We had ~$428k remaining at the end of FY23. The remaining funds were due to delay in finding and hiring post-doctoral appointees until later in FY22. Both Post-Docs ended their appointments in FY24-Q4. This took care of funding from Phase I. We received funding for Phase 2 in FY24 and have begun working on the proposed deliverables.

ML TOOLS FOR GAMMA-RAY TRACKING

AI/ML for the new generation of γ-ray tracking array :
Improve the current performance



Resolving power:
R~ Efficiency* PT/FWHM

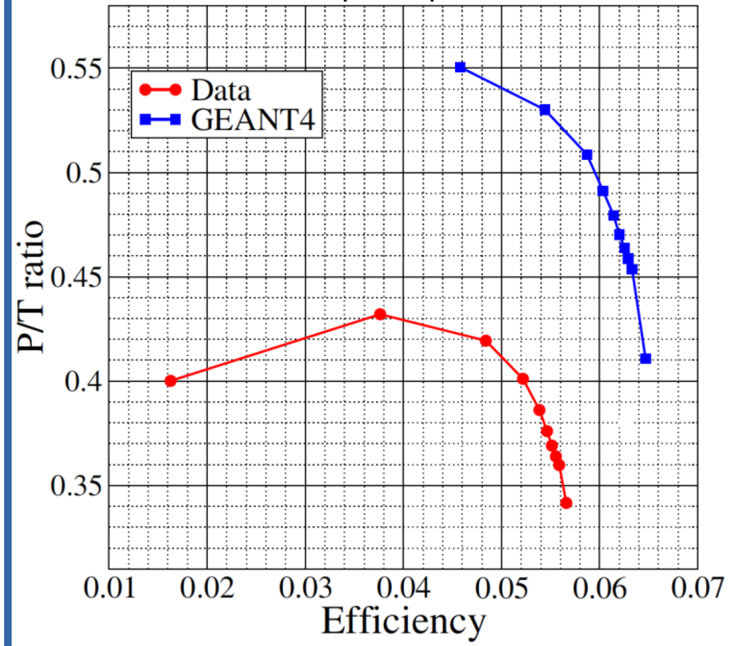
A Metric for the array performance

Benefit to the ATLAS program : GRETINA is frequently hosted at ANL
Very Important when GRETA will be in area 4 at Argonne

PROJECT GOALS

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

Curent tracking arrays (AGATA & GRETINA) do not meet the required performance



A. Korichi and T. Lauritsen, Eur. Phys. J. A (2019) 55: 121
AGATA-GRETINA Review paper

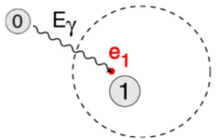
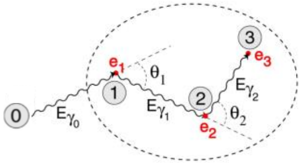
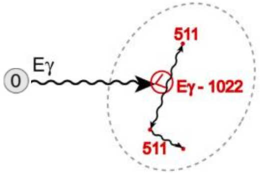
- Develop new techniques to enhance existing γ-ray tracking algorithms, boosting photopeak efficiency and improving the signal-to-background ratio (P/T).
- Adapt these techniques to accurately perform Doppler correction with the first interaction point (ordering!)
- Expand these methods to handle pair production events.
- Incorporate these tools into tracking codes used by the community.

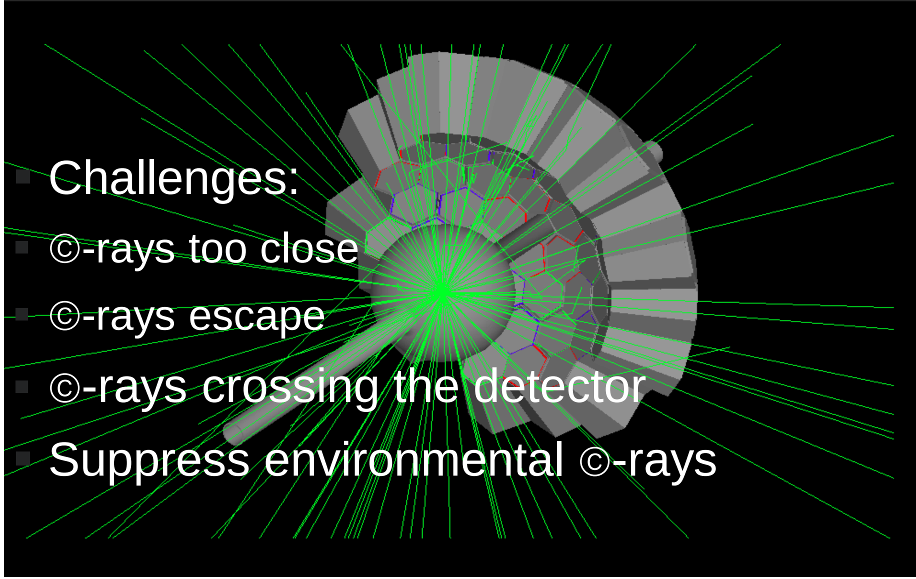
©-RAY TRACKING

Overview of the principle

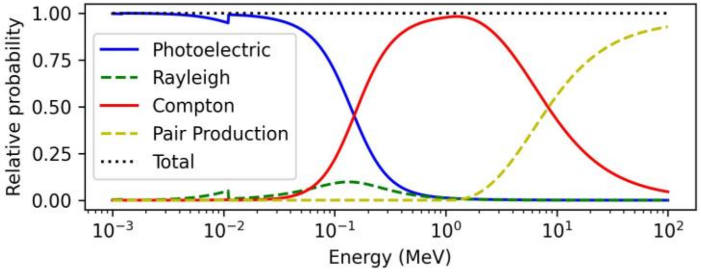
Three known interaction types of interest

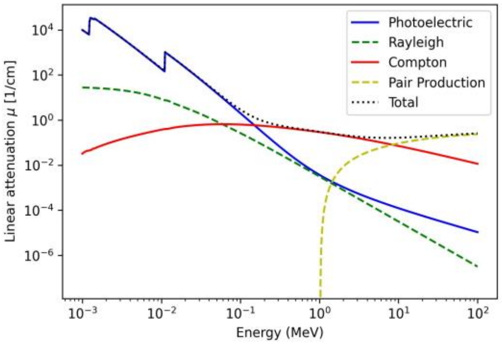
~ 100 keV | ~1 MeV | ~10 MeV | γ-ray energy

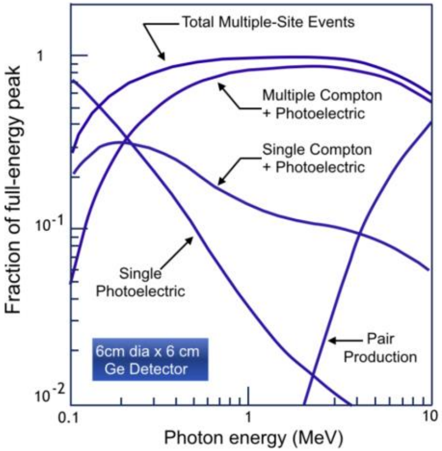
Photoelectric	Compton Scattering	Pair Production
		
Isolated hits	Angle/Energy	Pattern of hits
Probability of Interaction depth	$E'_\gamma = \dfrac{E_\gamma}{1 + \frac{E_\gamma}{m_0 c^2}(1 - cos\theta)}$	$E_{1st} = E_\gamma - 2m_0c^2$



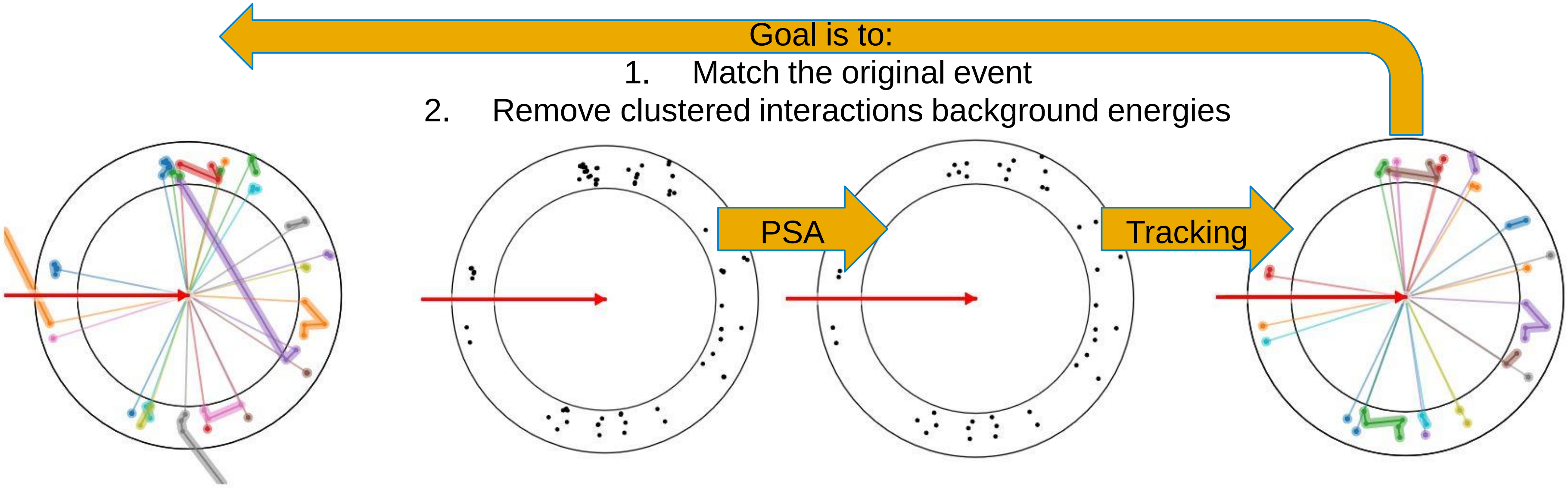
- Challenges:
- ©-rays too close
- ©-rays escape
- ©-rays crossing the detector
- Suppress environmental ©-rays







Goal of Tracking



Actual event: clustering/ordering of interactions

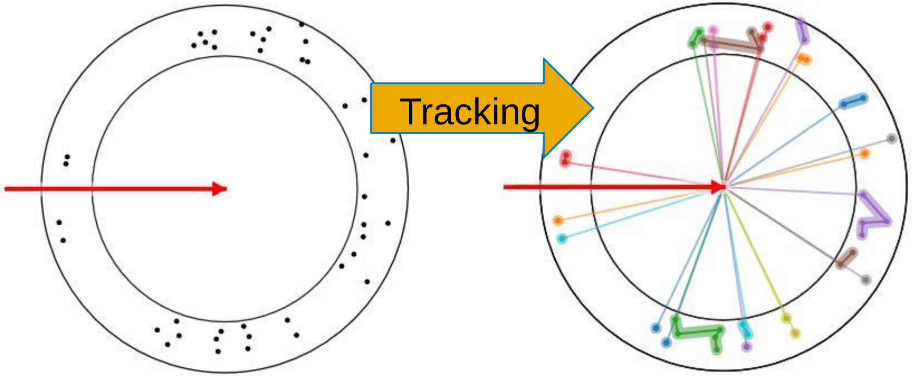
Actual interactions

Interactions recorded by PSA: "Packed and smeared"

Tracked event: interactions are clustered and ordered

The Full Tracking Problem

Organize interactions to recover the experimental event as best as possible



DATA: interaction positions and energies

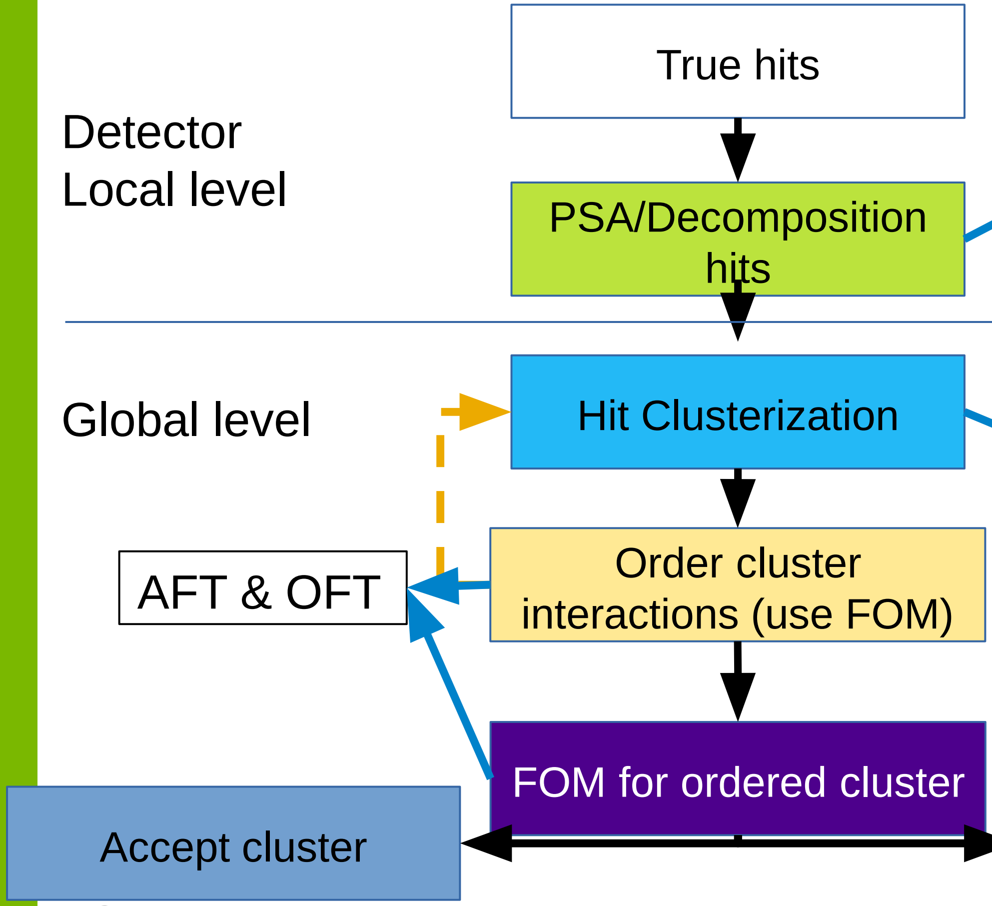
GOAL: Find the ordered clusters of interaction that optimize a *Figure of Merit (FOM)*

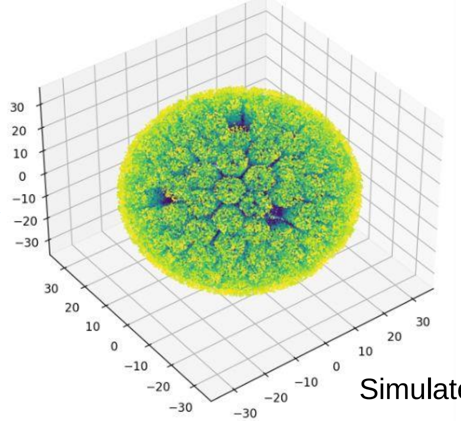
What FOM recovers the event?

PROBLEM: Too many possible ordered clusters of interactions!

10 interactions → 58,941,091 possible ordered clusters
60 interactions → as many possibilities as atoms in the universe

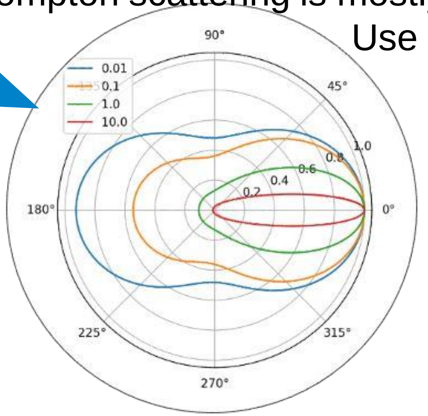
In Practice: Cluster then Order



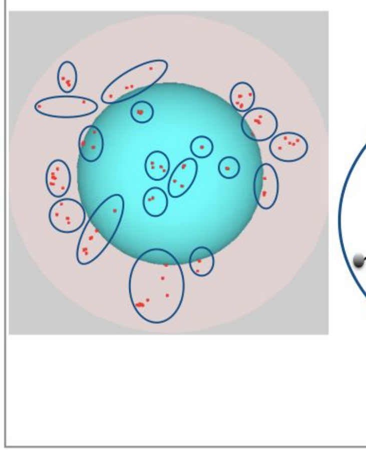


Simulated AGATA data

Compton scattering is mostly forward (Klein-Nishina)

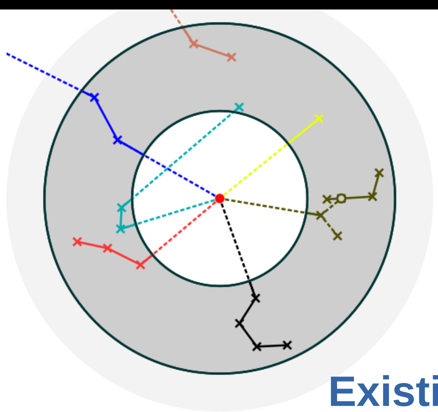


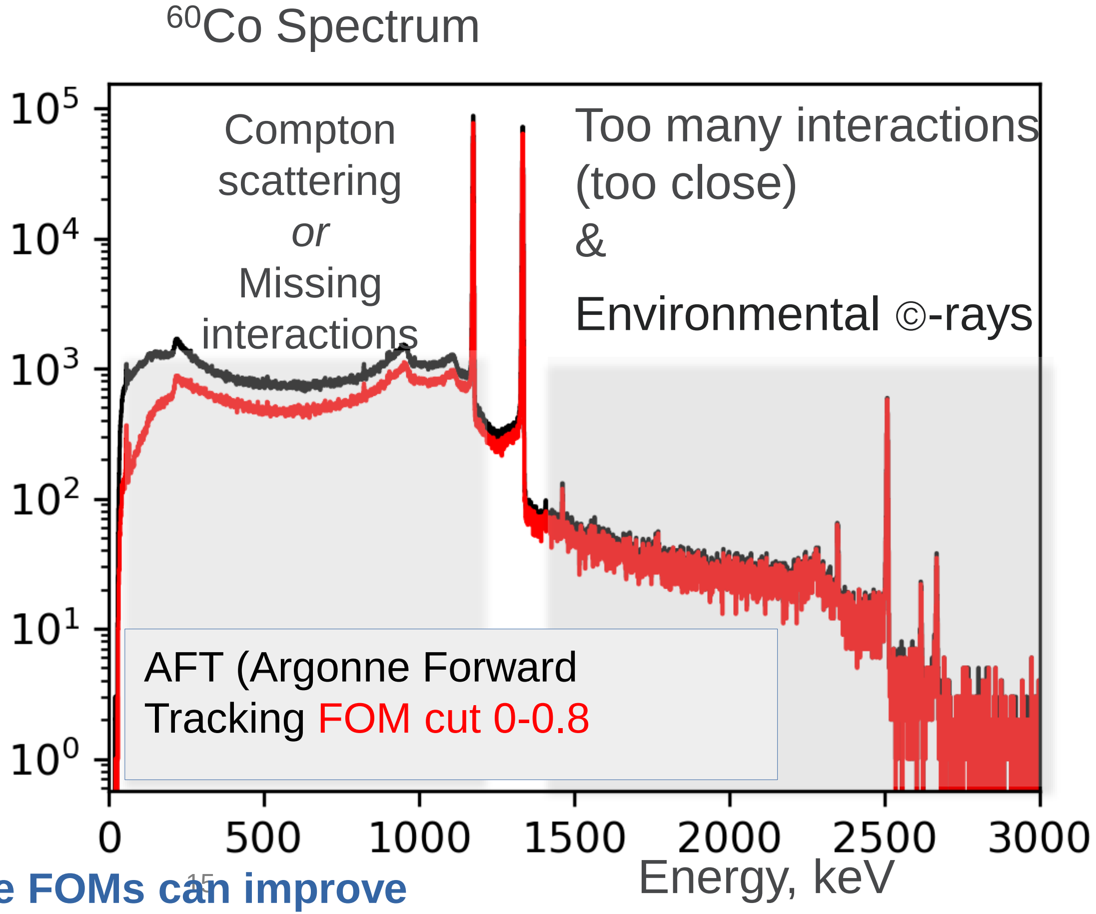
Use a cone clustering (alpha)



In Practice: with current algorithms

- Challenges:
- ©-rays too close
- ©-rays escape
- ©-rays crossing the detector
- Suppress environmental ©-rays



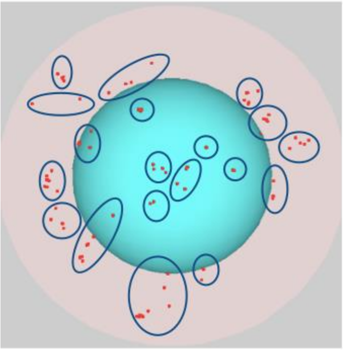


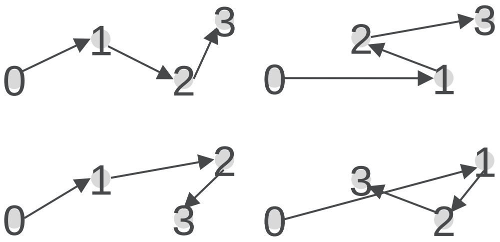
Existing possible FOMs can improve

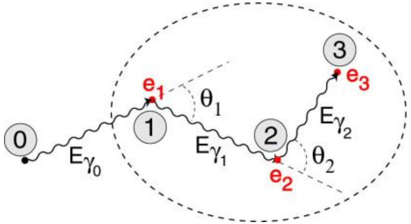
ML TOOLS FOR GAMMA-RAY TRACKING

Three complex operations

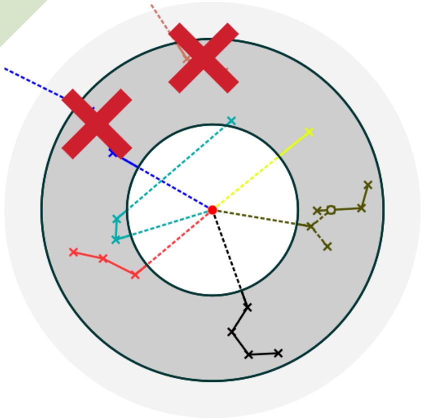
- Cluster interactions into separate γ-rays
- Order interactions for individual γ-rays
- Suppress γ-rays scattering out of the detector







3! = 6 permutations
For 3 interactions !



ADOPTED METHODOLOGY

- GEANT4 Simulated data
- Radioactive source data with GRETINA
- In-beam GRETINA data

High and low multiplicity data: clusterization, escape suppression
Efficiency and P/T evaluation

High and low recoil velocity: ordering the interactions
1st interaction for Doppler correction
1st and 2nd interactions for Linear polarization

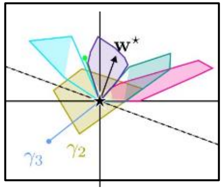
In all cases the results were compared to those obtained using conventional tracking codes AFT (Argonne Forward Tracking) and OFT (Orsay Forward Tracking)

ADOPTED METHODOLOGY

ML Approach for Learning-to-rank

- When ordering, we want

  FOM(best incorrect order) > FOM(true order)
- We don't care about the FOM value, only the difference between desired and undesired orders
- The **best incorrect order** requires ordering with the FOM
- Let FOM be weighted sum of physics derived objectives (e.g. existing FOMs), a simple, interpretable model, that prevents overfitting (*maximizes likelihood that the model can survive the translation from simulated to experimental data*



$$\textbf{FOM(order)} = \mathbf{w}^T \boldsymbol{f}\textbf{(order)}$$

- Allows simplification

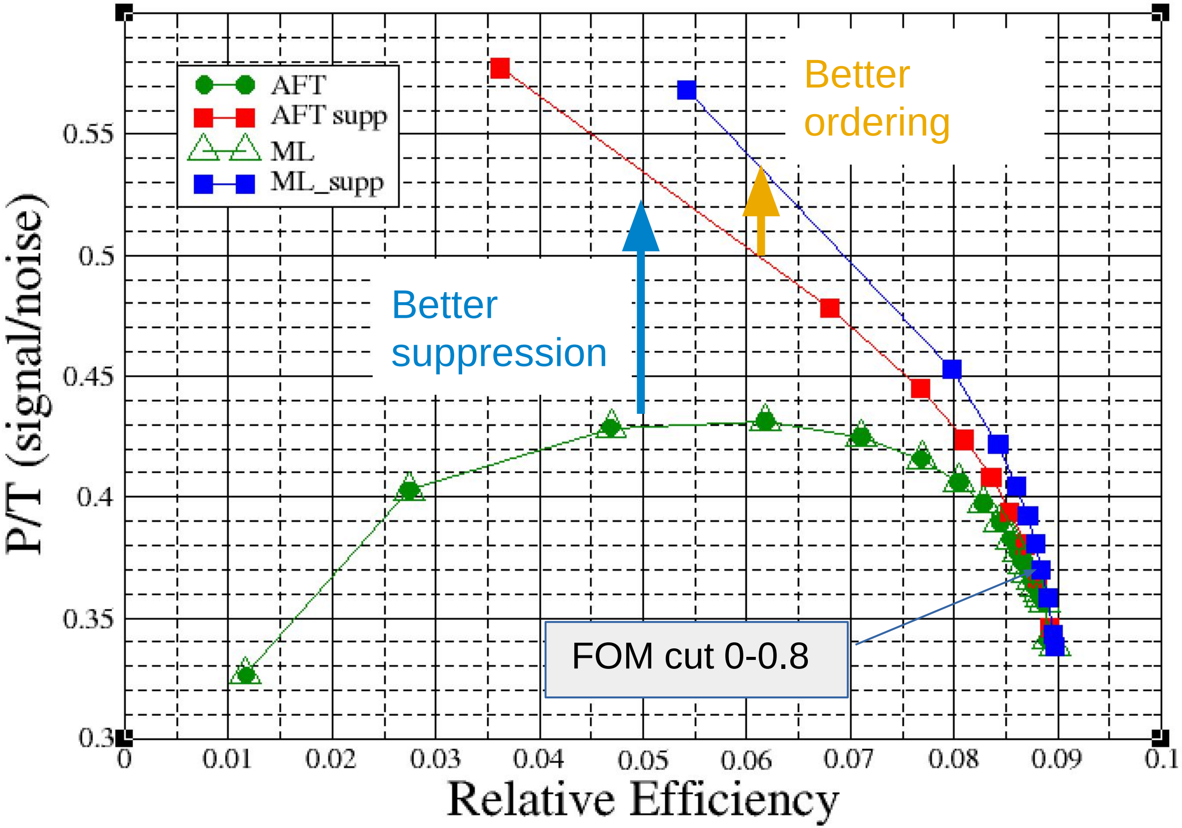
$$\mathbf{w}^T(\boldsymbol{f}\textbf{(incorrect)} - \boldsymbol{f}\textbf{(true)}) > 0$$

- If all features/FOMs are quantities that we want to minimize, constrain **w** positive, protect against overfitting
- Use linear classification (introduce mirrored data as second class → off the shelf solvers)

Results for Co source data

GRETINA (AFT) FOM

$$\frac{1}{N-1}\sum_{i=1}^{N-1}\left(\theta^{\text{geo}} - \theta^{\text{theo}}(E_{i-1}, E_i)\right)^2$$



Final FOM

Check to remove background

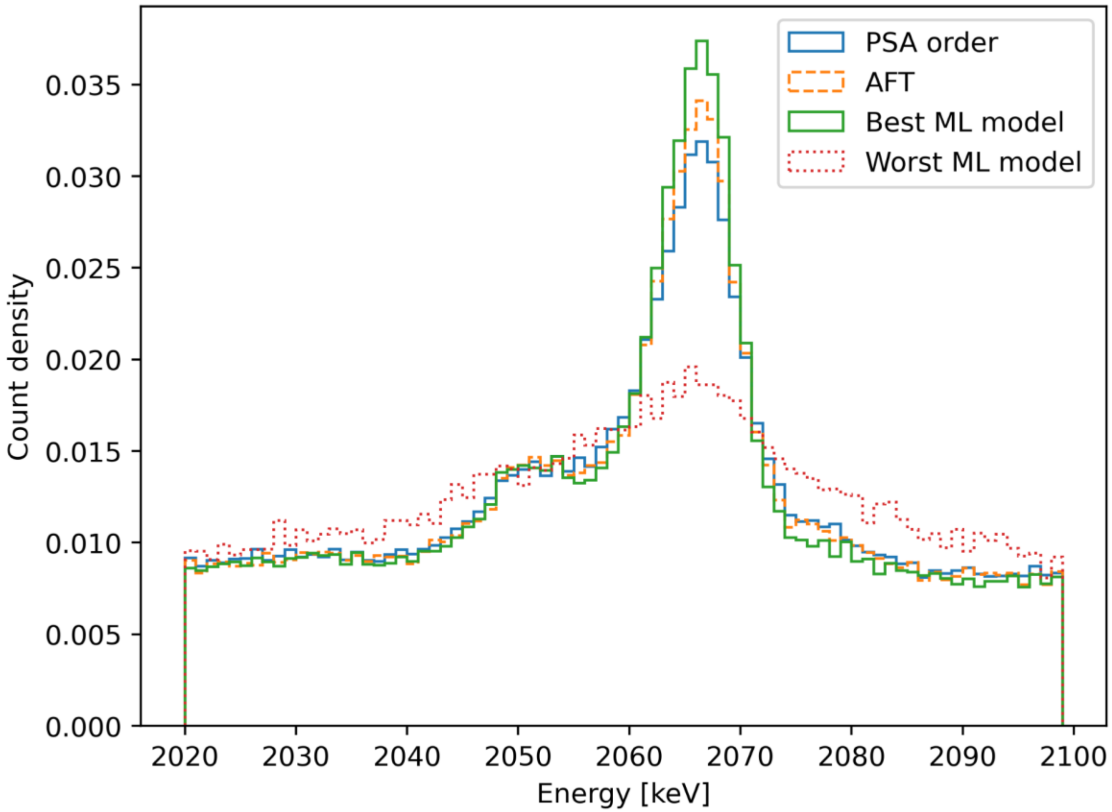
ML classification problem

Use linear model to help interpretability, protect against overfitting, help transition to experimental data

Good ordering, especially for incomplete gamma-rays, helps clean up the spectrum

NB: We need to simultaneously maximize the efficiency & the P/T

Results for ^{92}Mo in-beam data



Fusion-evaporation reaction

$^{12}C(^{84}Kr,xn)$

Beam Energy = 394 MeV

Recoil velocity ~8 %

No FOM cut/supression. Only Doppler correction

Example of parameters, FOMs and models that have been used in this work

A	B	Simulated data			Experimental data			I	J
		all_accuracy_correlation	all_accuracy_R	complete_accuracy_correlation	complete_accuracy_R	incomplete_accuracy_correlation	incomplete_accuracy_R	validation_accuracy_	validation_accuracy_R
C	C_1000	-0.058193674	0.058193674	-0.053454752	0.053454752	-0.052224147	0.052224147	0.20516106	0.00045849
	C_10000	0.058193674	0.058193674	0.053454752	0.053454752	0.052224147	0.052224147	-0.20516106	0.00045849
Columns	**cols_aft**	-0.076325647	0.076325647	-0.005300437	0.005300437	-0.204519661	0.204519661	-0.01204583	0.8387107
	cols_aft-fast	0.0888634	0.0888634	0.107414741	0.107414741	0.025623966	0.025623966	0.0385706	0.5144265
	cols_aft-fast-tango	0.128330901	0.128330901	0.109293607	0.109293607	0.133188852	0.133188852	0.07734063	0.19061326
	cols_aft-fastest	0.021426865	0.021426865	0.052850234	0.052850234	-0.050385041	0.050385041	-0.14379215	0.01459295
	cols_aft-fastest-tango	0.069065148	0.069065148	0.063813769	0.063813769	0.061197885	0.061197885	-0.07738052	0.19038397
	cols_aft-tango	-0.006229761	0.006229761	-0.003607784	0.003607784	-0.010028997	0.010028997	-0.07953441	0.1783003
	cols_aft-true	-0.432470377	0.432470377	-0.203709027	0.203709027	-0.794319516	0.794319516	0.08811009	0.13578374
	cols_all	0.157322643	0.157322643	0.126755755	0.126755755	0.178449978	0.178449978	0.36398759	0
	cols_fast	0.089000176	0.089000176	0.107563293	0.107563293	0.025698618	0.025698618	-0.06284176	0.28783962
	cols_fast-tango	0.128222102	0.128222102	0.109299883	0.109299883	0.132868287	0.132868287	0.05580173	0.3453722
	cols_fastest	-0.520524263	0.520524263	-0.620266848	0.620266848	-0.168822785	0.168822785	-0.13266372	0.02435088
	cols_oft	0.113075771	0.113075771	0.104667581	0.104667581	0.099797409	0.099797409	0.09618718	0.10330652
	cols_oft-fast	0.153309525	0.153309525	0.137876211	0.137876211	0.143771884	0.143771884	0.00680071	0.90851543
	cols_oft-fast-tango	0.16630786	0.16630786	0.13366864	0.13366864	0.189327228	0.189327228	-0.038431	0.51595111
	cols_oft-fastest	0.130196021	0.130196021	0.11340284	0.11340284	0.129833899	0.129833899	-0.06679056	0.25855802
	cols_oft-fastest-tango	0.140003446	0.140003446	0.10277407	0.10277407	0.179850803	0.179850803	-0.05422619	0.35918367
	cols_oft-tango	0.129167097	0.129167097	0.093509465	0.093509465	0.168679336	0.168679336	-0.05350823	0.36559044
	cols_oft-true	-0.478740905	0.478740905	-0.530005993	0.530005993	-0.240212145	0.240212145	-0.00558416	0.92482719
Model type	model_type_lp	0.043636361	0.043636361	0.038356837	0.038356837	0.042782798	0.042782798	0.06523047	0.26987133
	model_type_lr	-0.077810651	0.077810651	-0.06480834	0.06480834	-0.0838193	0.0838193	0.12590334	0.03269045
	model_type_milp	0.099322254	0.099322254	0.08493778	0.08493778	0.102348504	0.102348504	-0.23708948	0.00004821
	model_type_svm	-0.065147964	0.065147964	-0.058486277	0.058486277	-0.061312002	0.061312002	0.04595567	0.43721044
Non-negative	nonneg_False	0.00252598	0.00252598	-0.032721003	0.032721003	0.075811971	0.075811971	-0.30128662	0.00000019
	nonneg_True	-0.00252598	0.00252598	0.032721003	0.032721003	-0.075811971	0.075811971	0.30128662	0.00000019

C: Controls the sparsity of the model; a smaller C means a simpler model

Columns: Groups of FOM features

Model type: The approach for training the ML model

LP: Linear program (more precise than SVM), LR: Logistic regression (simplest, but least accurate)

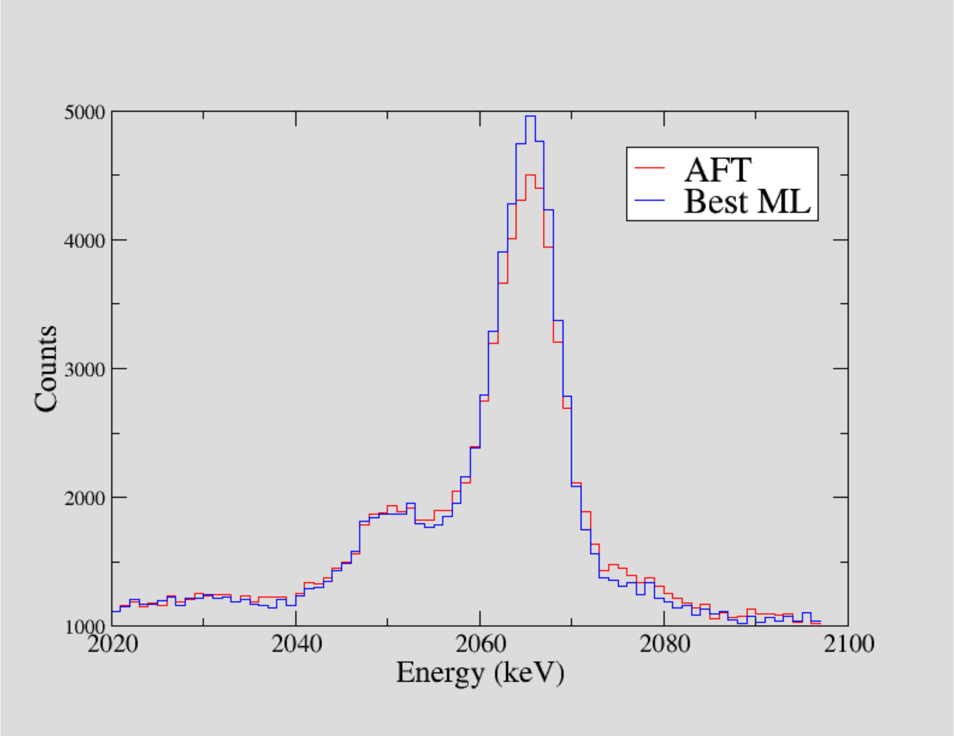
MILP: Mixed integer linear program (most accurate), SVM: Support-vector machine (basic linear model)

Non-negative: If "noneg = True," all weights in the FOM are non-negative, focusing on minimizing values.

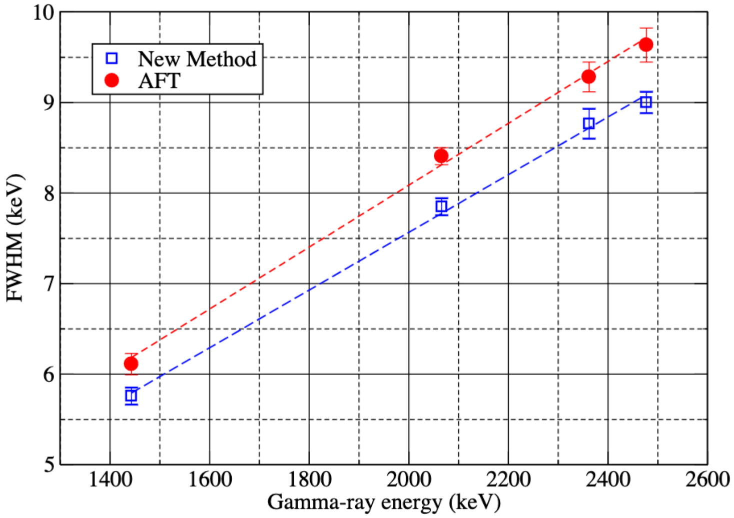
If "noneg = False," some weights can be negative, allowing for maximization.

Results for ^{92}Mo in-beam data

Experiment performed at ATLAS (for the evaluation of GRETINA performance)



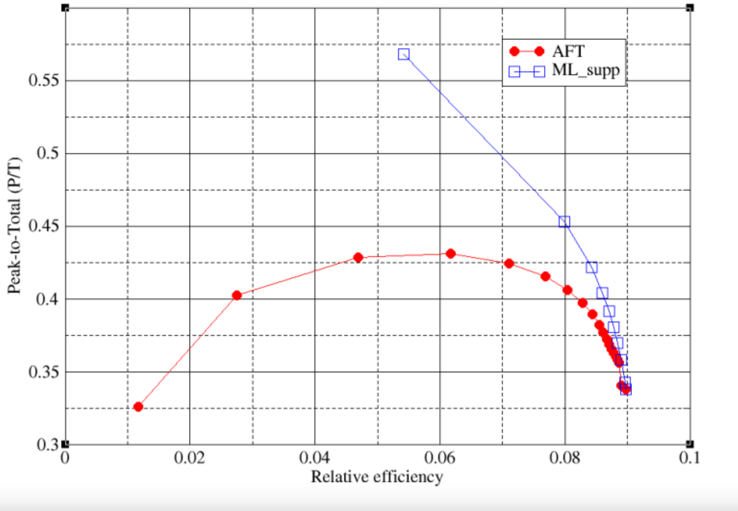
FWHM	Peak Area	Energy
8.02(6)	31763(266)	2065.63(4)
8.75(7)	30169(277)	2065.65(5)



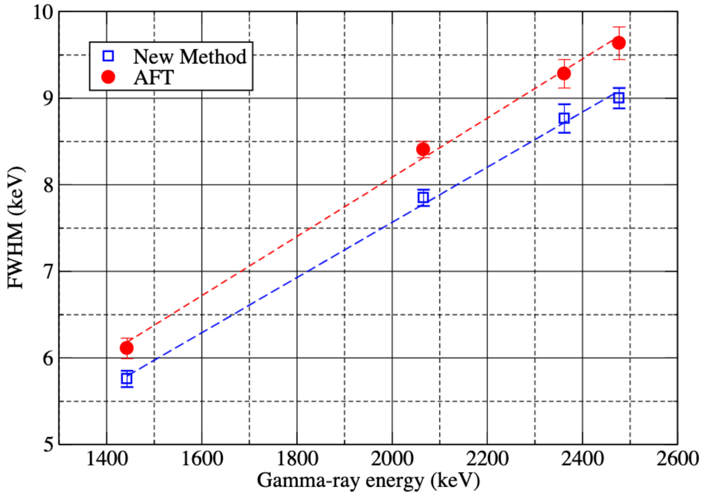
Clear improvement in the energy resolution & efficiency

Results summary

P/T improved by ~10 %
Efficiency ~ 6 %



FWHM improved by 9 %



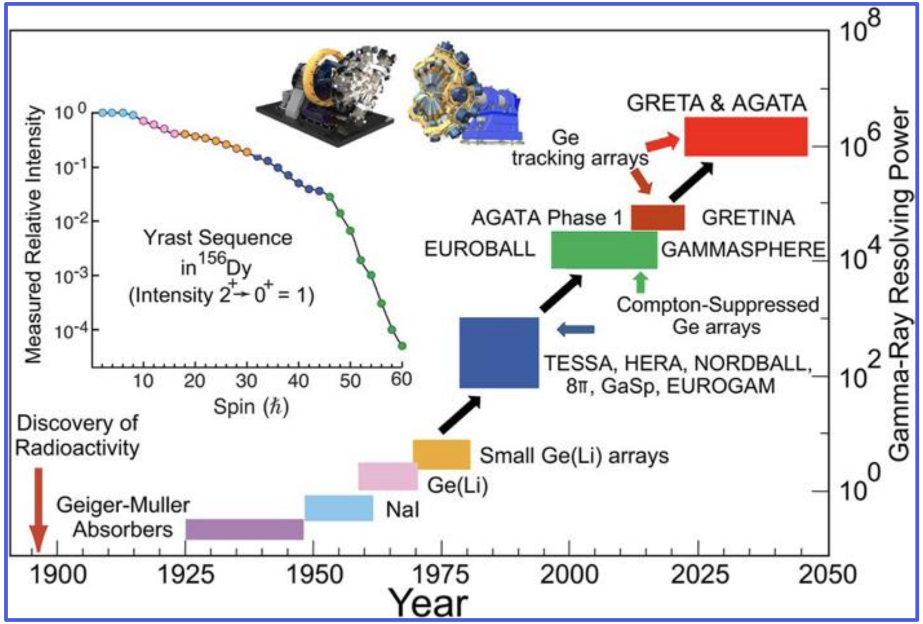
These numbers look small BUT !

FIGURE OF MERIT FOR THE EVALUATION OF A SPECTROMETER PERFORMANCE
COMPOSITE PARAMETER WITH:

Total photopeak efficiency ∑
Energy resolution FWHM
photopeak-to-total ratio P/T

$$R \sim \frac{\varepsilon \ \text{™}E}{FWHM} \ P/T$$

™E Average spacing between consecutive transitions in a typical cascade



Resolving Power(RP) ~ R^{Fold}

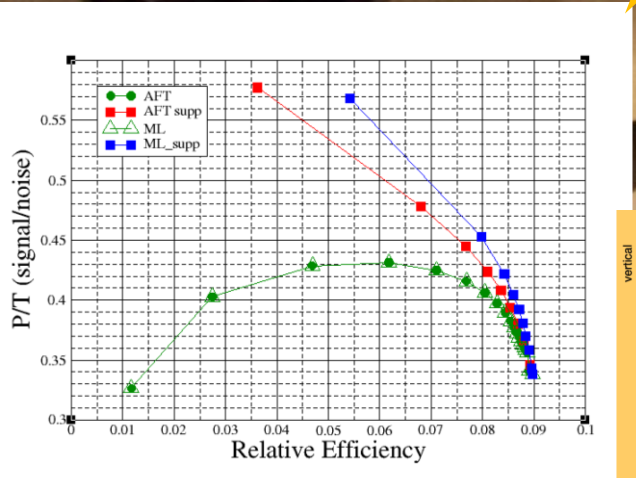
For a 5-fold ©-ray event
(typical for high-spin Gammasphere exp.)

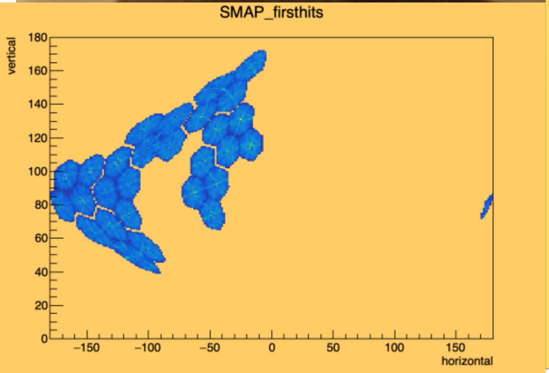
10 %P/T better → increase RP by 60%

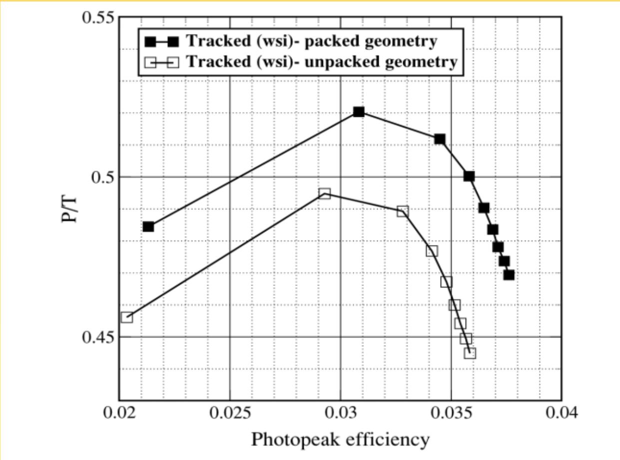
8 % fwhm better → increase RP by 52%

This results in more than a factor 2.5 gain in the Resolving Power

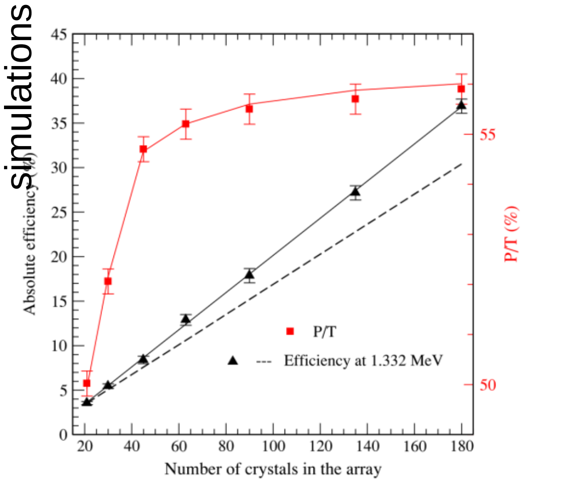
Excellent with a less than optimal array configuration







GEANT4 simulations

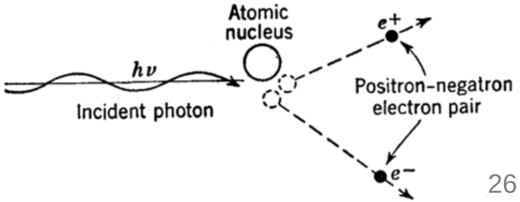


A more populated array towards GRETA (with new PSA?)will do much better !

GAMMA-RAY TRACKING SUMMARY

- **Current project milestones, (nearly complete)**
  - Python Code has been published on GitHub
  - New ordering approaches enhance existing techniques, improving the resolving power by up to 2.4 for Doppler-corrected data
  - Learning To Rank (LTR) methods enable expanded tracking optimizations
  - New suppression approaches further enhance the resolving power and are nearly ready for experiments
  - Journal paper manuscript is in preparation

- **Renewal project milestones (continuing)**
  - Pair production tracking for higher energy (>7 MeV) gamma-rays



github.com/lynntf/GRETO

Gamma Ray Energy Tracking Optimization

Deliverable

Lately optimized for speed

12h→ 2h (Moly data)

GAMMA-RAY TRACKING CONCLUSION

- Current project milestones are nearly complete.

The synergy/collaboration between the Physics Division and the MCS Division has been crucial to the project's success.

Thomas Lynn's dedicated efforts and expertise have been indispensable. He is the main player!

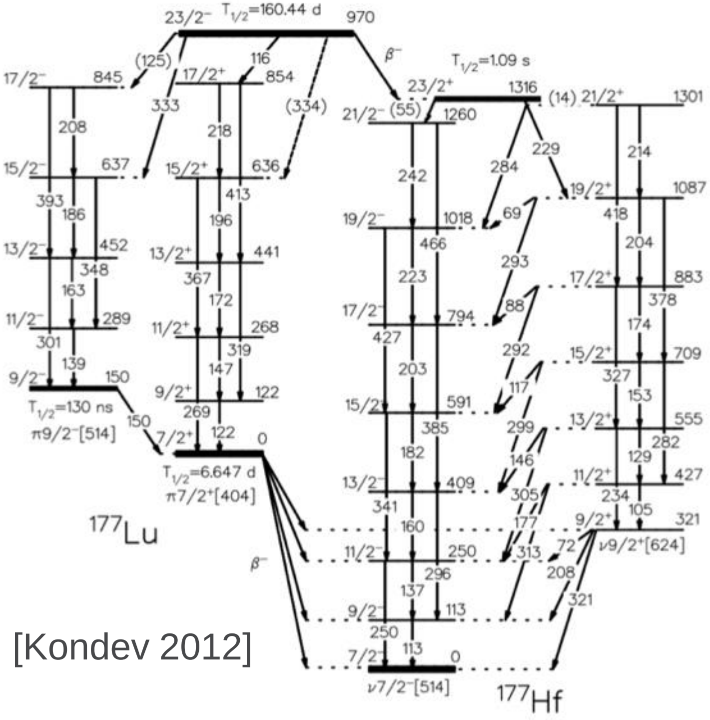
Thank you !

ML TOOLS FOR LEVEL-SCHEME DESIGN

MAPPING OF EXCITED STATES IN NUCLEI

Building level schemes from data collected from the large gamma-ray arrays

- A major deliverable from large γ-ray arrays is the mapping of excited nuclear states.
- Accomplished by analysis of γ-ray coincidence data *e.g*. 2-fold, 3-fold, …
- Level schemes can be complicated, and analysis times can take many months.
- Can we develop tools to speed up analysis and quantify accuracy?



[Kondev 2012]

ML TOOLS FOR LEVEL-SCHEME DESIGN

Overview of Inverse Optimization Approach

Single, Doublet, or Triplet Data → **Optimize Transitions** → **Represent as Level-Scheme**

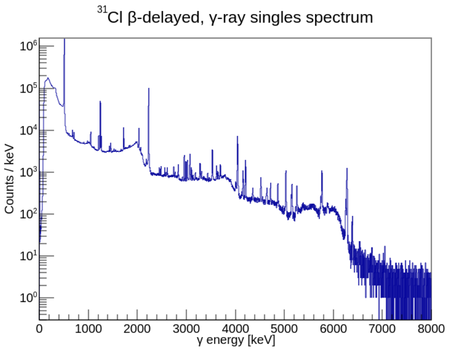
- Data preparation
- Extraction tools for coincidence data

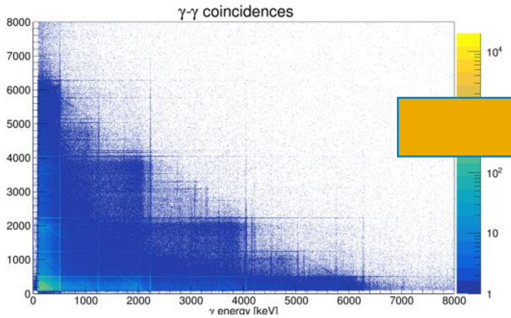
- Inverse optimization to determine transitions
- ML-based optimizers

- Graph-based level-scheme generation
- ML-based extensions

Part I: Software Tools for Spectroscopic Analysis

- **Goal: Develop user-friendly software tools to streamline the process of analyzing large datasets from gamma-ray spectroscopy experiments**
- **Extract intensities from 1D singles and 2D coincidence spectrum which can be used to reconstruct nuclear level scheme**



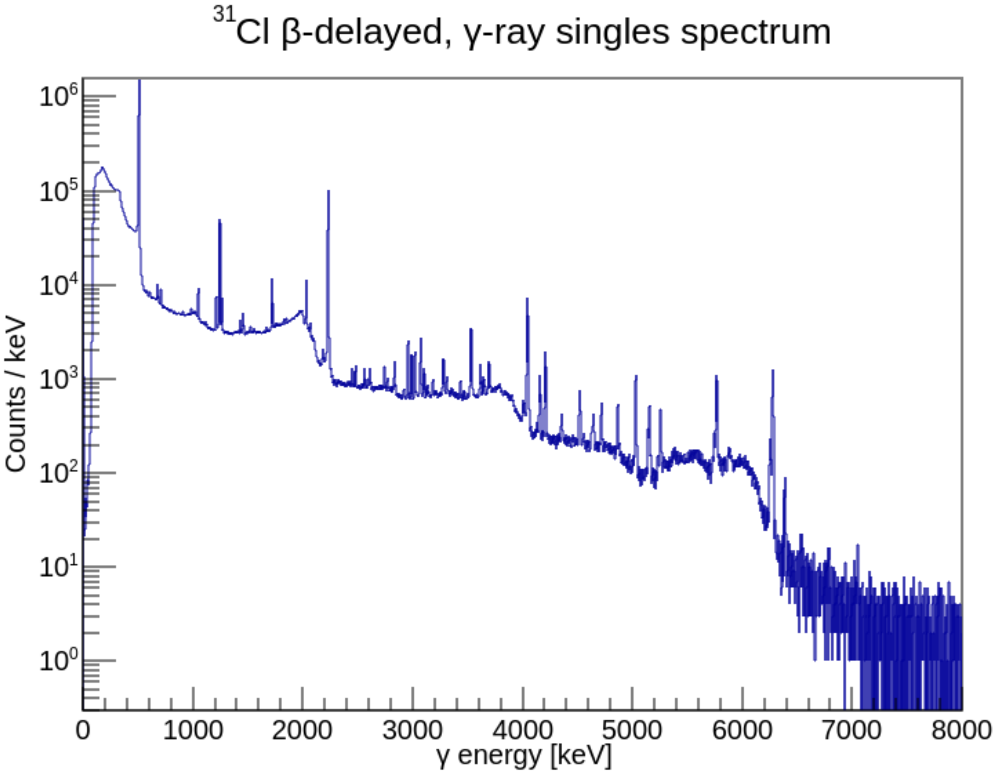


$$S = \begin{pmatrix} S_1 \\ S_2 \\ \cdots \\ S_n \end{pmatrix} \qquad C = \begin{pmatrix} 0 & C_{i,j} & \cdots & C_{i,j} \\ C_{i,j} & 0 & & \vdots \\ \vdots & & 0 & \\ & & & \ddots \\ C_{i,j} & \cdots & & 0 \end{pmatrix}$$

1D Gamma-Ray Singles Spectrum

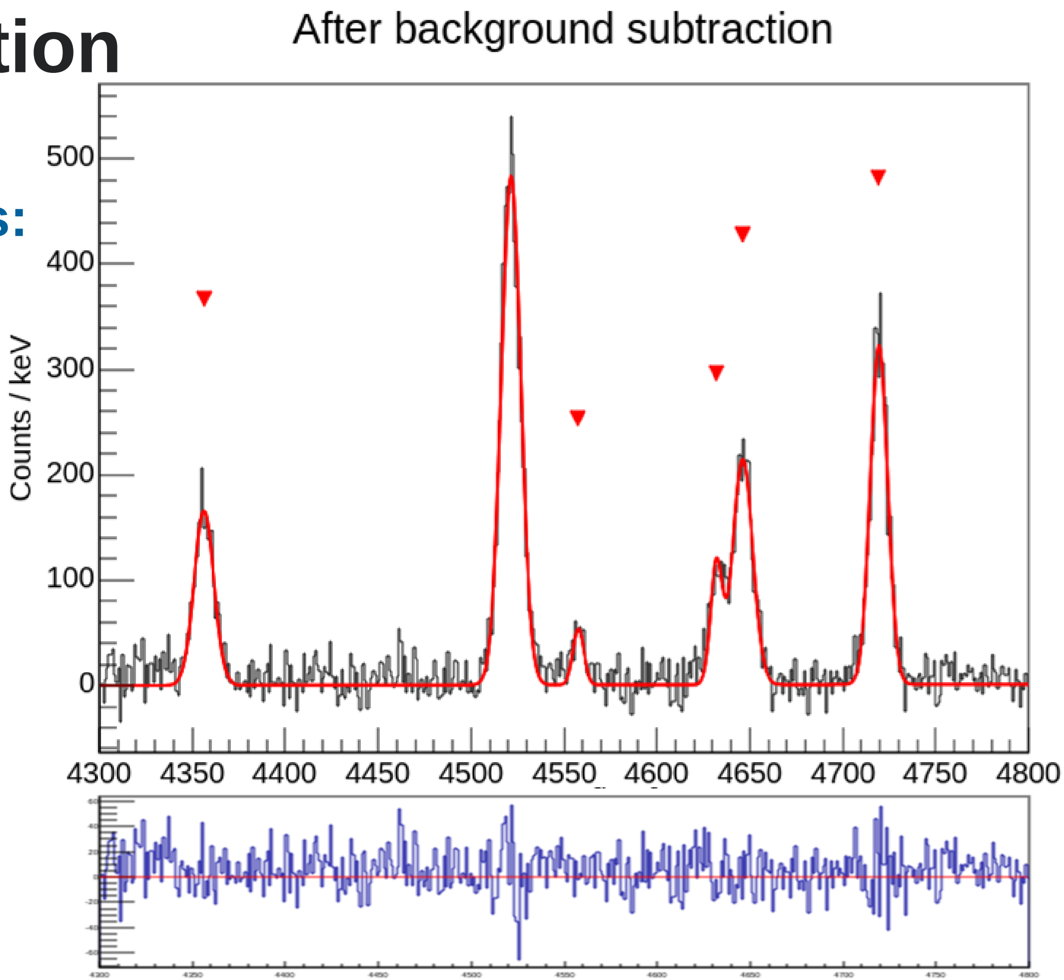
- **All statistics for *n* total γ transitions as measured by spectrometer**
- **The intensity of the i^{th} γ-ray transition is stored as S_i in vector *S***

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



Background Subtraction and Peak Fitting

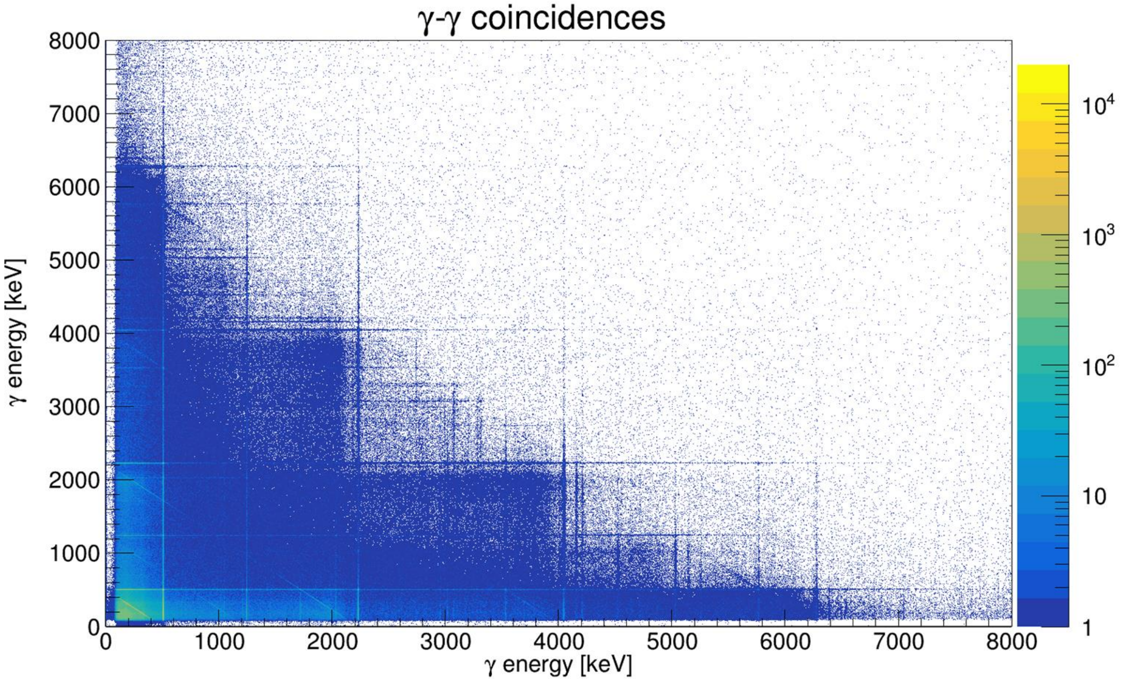
- **Extract energies/intensities:**
  - **Subtract background histogram**
  - **Estimate remaining background with polynomial function**
  - **Fit peaks with Gaussian distributions**
- **Additional options:**
  - **Plot residuals**
  - **Manually add peaks**
  - **Constrain peak shape**



Gamma-Gamma Coincidence Matrix

- The number of γ_i-γ_j coincidences is stored in each element $C_{i,j}$ within the reduced coincidence matrix C
- The matrix is symmetric $C_{i,j} = C_{j,i}$ because there is no information about the order of the cascade

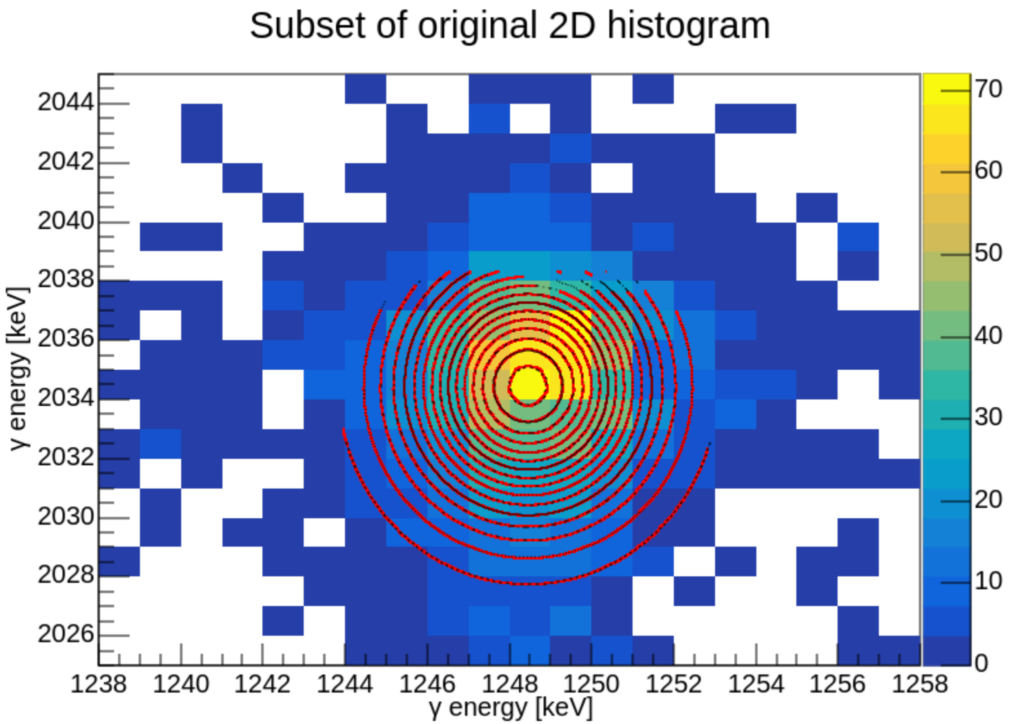
$$C = \begin{pmatrix} 0 & C_{i,j} & \cdots & C_{i,j} \\ C_{i,j} & 0 & & \vdots \\ \vdots & & 0 & \\ & & & \ddots \\ C_{i,j} & \cdots & & 0 \end{pmatrix}$$



2D Coincidence Spectrum Fitting

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

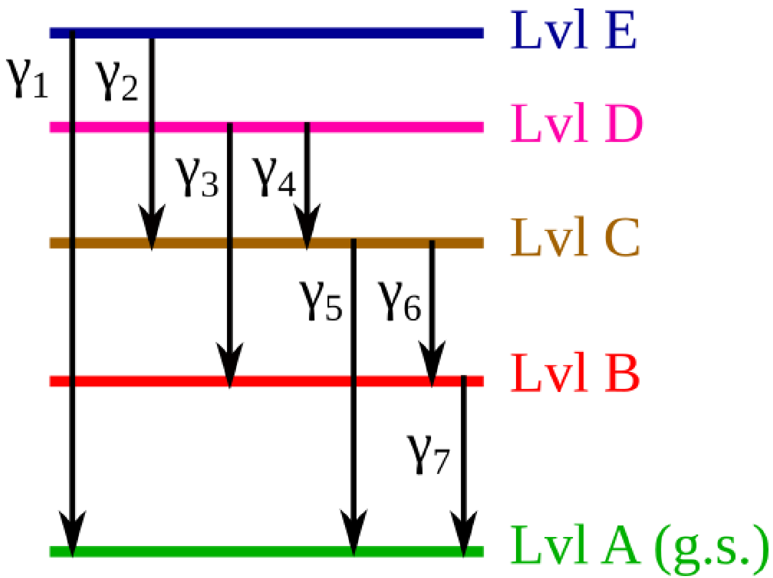
- **Use information from the γ-ray combined singles spectrum as well as the background-subtracted, γ-gated coincidence spectrum to populate the undirected coincidence matrix C**
- **Automatic fitting procedure using 2D Gaussian distribution**



Part II: Numerical Optimization for Level Scheme Building

- **Goal: Numerically solve a system of matrix equations containing experimental data in order to reconstructed an ordered nuclear decay scheme diagram**

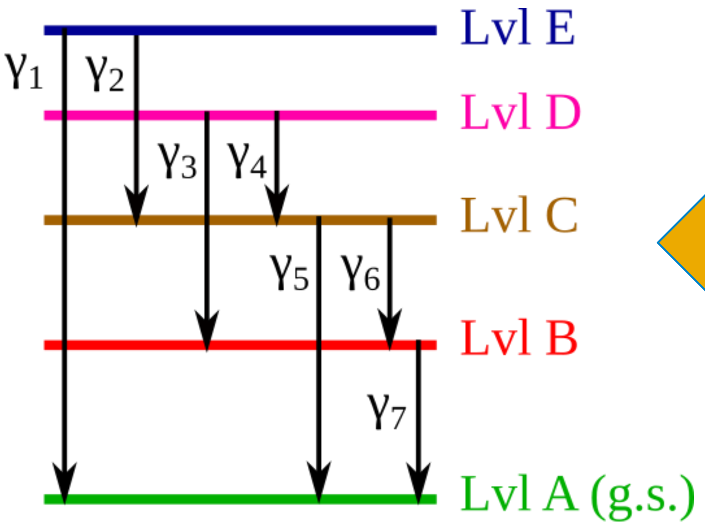
$$S = \begin{pmatrix} S_1 \\ S_2 \\ \cdots \\ S_n \end{pmatrix} \qquad C = \begin{pmatrix} 0 & C_{i,j} & \cdots & C_{i,j} \\ C_{i,j} & 0 & & \vdots \\ & & 0 & \\ \vdots & & \ddots & \\ C_{i,j} & \cdots & & 0 \end{pmatrix}$$

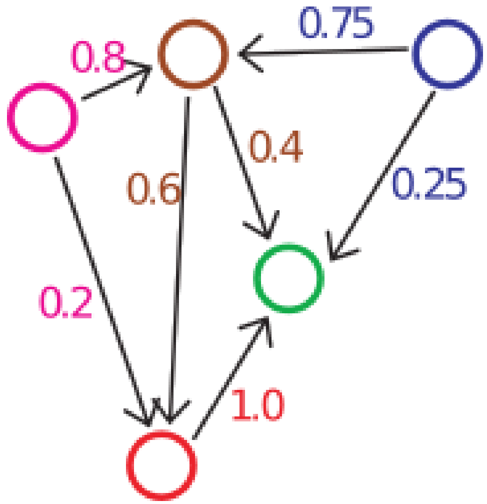


“Level-Centric” Decay Scheme

Decay schemes can be represented as graphs.

- Each level within the decay scheme corresponds to a vertex (or node), and the edges connecting these vertices correspond to γ-ray transitions between levels.
- Gamma-ray branching ratios correspond to edge weights.



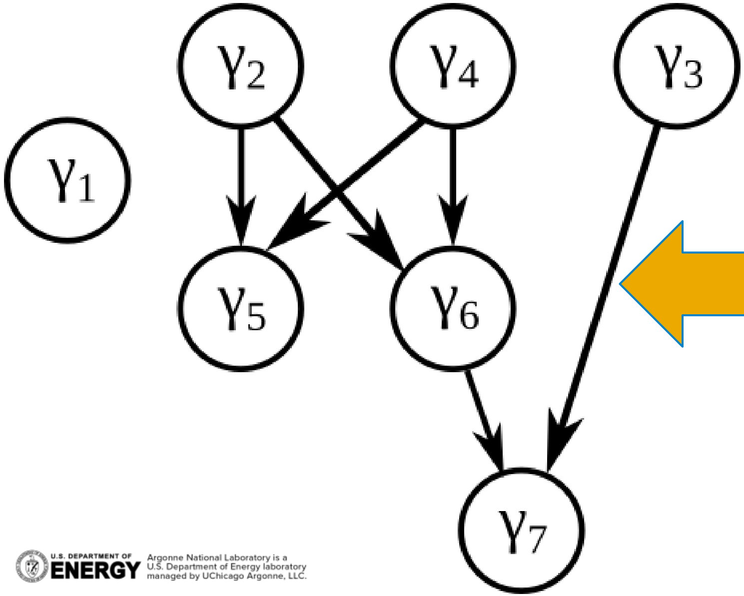


G. Demand, *Development of a Novel Algorithm for Nuclear Level Scheme Determination*, Master’s thesis, University of Guelph, 2009.

Adjacency Matrix

Every weighted, directed graph has a unique adjacency matrix *A*.

- Given a start position of vertex *i*, element $A_{i,j}$ is the probability of transitioning directly to vertex *j* (non-zero numbers=branching ratios)
- Transition energy information not needed for network connectivity but is useful for level-centric scheme construction.



	γ_1	γ_2	γ_3	γ_4	γ_5	γ_6	γ_7
γ_1	0	0	0	0	0	0	0
γ_2	0	0	0	0	0.4	0.6	0
γ_3	0	0	0	0	0	0	1.0
γ_4	0	0	0	0	0.4	0.6	0
γ_5	0	0	0	0	0	0	0
γ_6	0	0	0	0	0	0	1.0
γ_7	0	0	0	0	0	0	0

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:

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

Solving an Inverse Problem

Numerical Solution

- We have two governing equations:

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

- Satisfying both equations leads to the nonlinear optimization problem:

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

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

PHYSICS!

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)

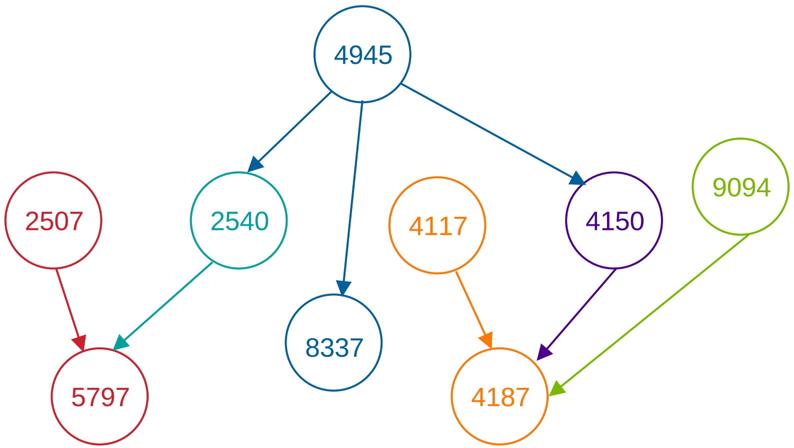
G. Demand, *Development of a Novel Algorithm for Nuclear Level Scheme Determination*, Master's thesis, University of Guelph, 2009.

Mapping Between Transition- and Level-Space

Reconstructing Level-Centric Decay Scheme from Adjacency Matrix

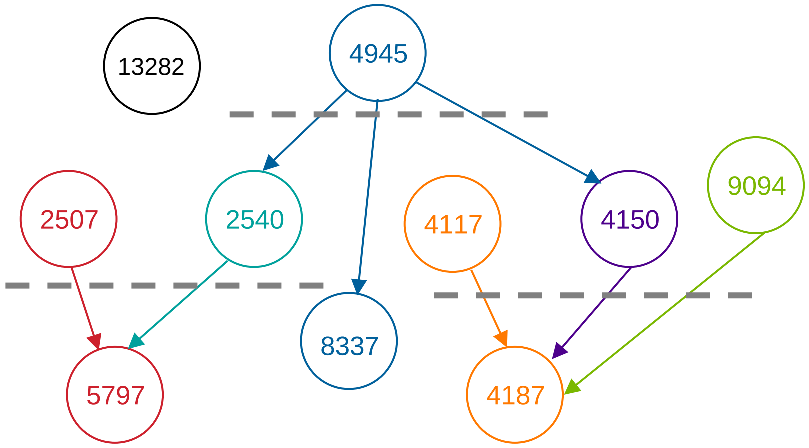
Adjacency =

	2507	2540	4117	4150	4187	4945	5797	8337	9094	13282
2507	0	0	0	0	0	0	1	0	0	0
2540	0	0	0	0	0	0	1	0	0	0
4117	0	0	0	0	1	0	0	0	0	0
4150	0	0	0	0	1	0	0	0	0	0
4187	0	0	0	0	0	0	0	0	0	0
4945	0	0.70	0	0.23	0	0	0	0.07	0	0
5797	0	0	0	0	0	0	0	0	0	0
8337	0	0	0	0	0	0	0	0	0	0
9094	0	0	0	0	1	0	0	0	0	0
13282	0	0	0	0	0	0	0	0	0	0

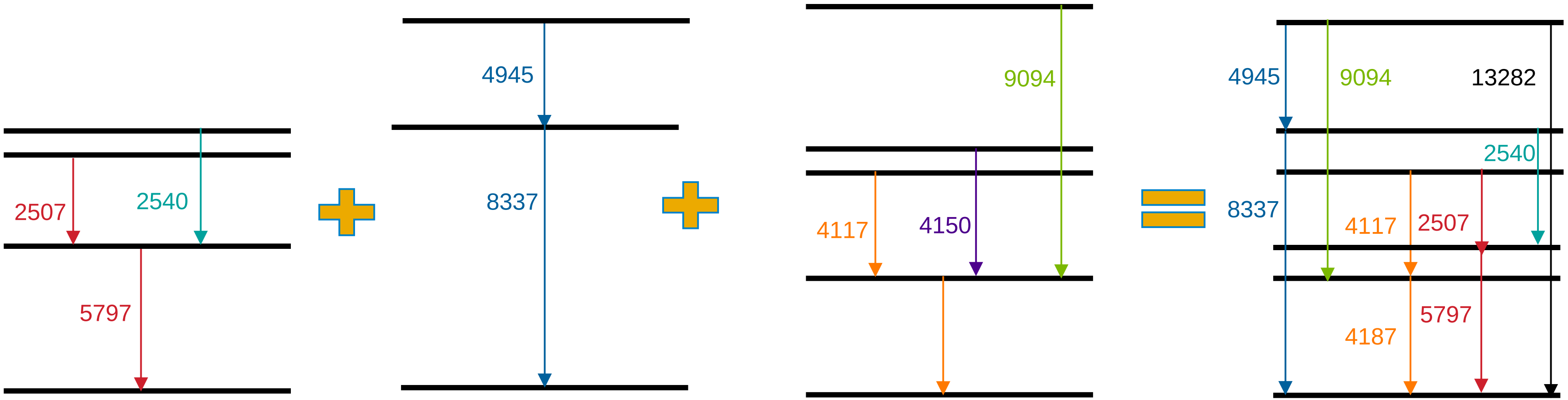


G. Demand, *Development of a Novel Algorithm for Nuclear Level Scheme Determination*, Master's thesis, University of Guelph, 2009.

Transition-centric graph



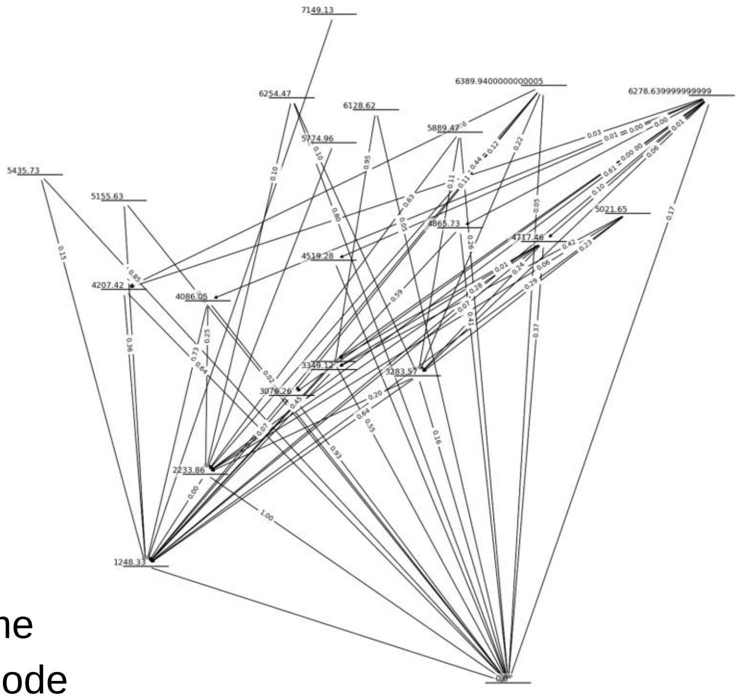
Level-centric decay scheme



Benchmarking our Work

Successful Outcomes

- Ipopt used to solve large-scale, nonlinear optimization problem
- Successful cases:
  - ^{20}O
  - ^{43}K
  - ^{182}Ta
  - ^{200}Pb
- Maxing out at about 30 - 40 transitions per decay scheme
- Time to converge <1 minute on a serial CPU compute node
- Example case: ^{200}Pb (20 transitions)
  - Original problem size: 800 variables, 390 constraints
  - Reduced problem size: 627 variables, 216 constraints



Benchmarking our Work

Potential Failures

1. Fails to converge on a solution within several hours; stop to check current "best guess"
   - Potential solution: parallelizing algorithm and utilize HPC resources
2. Converges to incorrect answer
   - Optimizer could converge to solution where function output is zero; if converges to solution but objective function is non-zero, decay scheme must be incorrect
   - Borderline cases where solution is an easy fix, i.e. a few misplaced, weak transitions

Potential Solutions

- Using prior information about decay scheme to constrain elements of adjacency matrix A to reduce parameter space in numerical optimization
- Pivot from nonlinear optimization to mixed-integer, linear optimization

Future Outlook

- Finish documenting Jupyter Notebook and publish open-source code for low-energy nuclear community to alpha test
- Add more user flexibility for background and peak modeling
- Expand numerical optimization test cases to real data
- Extend these techniques to 3D coincidence data (phase 2)

TABLE OF DELIVERABLES AND SCHEDULE

REMAINING MILESTONE SCHEDULE

Year	Milestone	Personal
FY25	Improve peak-to-total of γ -ray spectra	AK, TL
FY25	Accel. merging of DAQ data	RL, RR, TL
FY25	Algorithms to automatically extract inte	MC, FK
FY25	Optimization and ML tools for Coulex	MS, SL, DL
FY26	Improve tracking eff. at high energy	AK, TL
FY26	Storage of even in indexed form	RL, RR, TL
FY26	Level-scheme design from N-fold data	SL, MC, TL
FY25	Reinforced learning of Coulom excit.	MS, SL, DL

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Collaborators at Argonne National Laboratory

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And thank you for your attention!