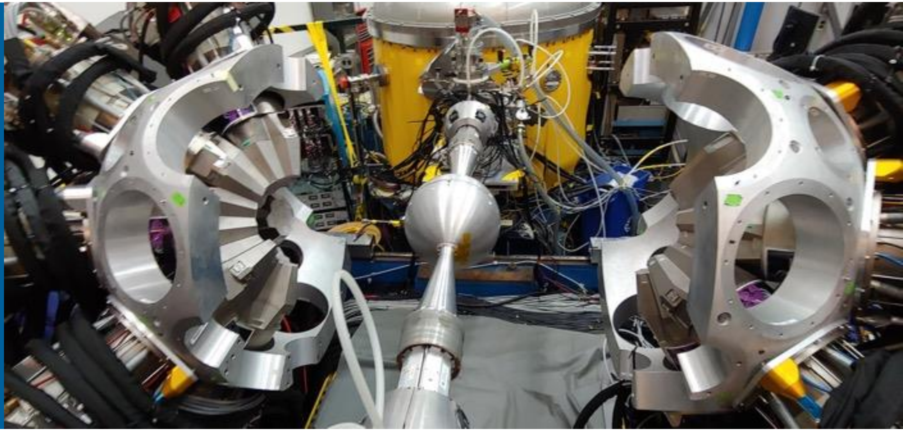
PRESENTATION TO NUCLEAR PHYSICS AI AND DATA SCIENCE, PI EXCHANGE MEETING

DEVELOPING MACHINE-LEARNING TOOLS FOR GAMMA-RAY ANALYSIS



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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 such Gammasphere, GRETINA and AGATA. Specifically, we are working on three closely related areas in which modern optimization models and tools together with machine-learning approaches will be deployed to provide an automated data-analysis workflow for these types of experiments, namely:

- Develop data preparation and workflow tools to quickly extract the required information from the gamma-ray data collected by the devices.
- Develop machine-learning tools to improve γ-ray tracking
- 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 intensity and background rejection.
- Develop 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.

Level Scheme Construction

- Develop tools to automatically extract intensity information from gamma-ray coincidence data.
- Using known level schemes, develop a mathematical toolkit to build levels schemes from the inputted data for both 2-fold and 3-fold coincidence information.
- Apply toolkit to both simulated data and experimental data taken with Gammasphere and GRETINA.

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 (Orsay Staff)**
- Torben Lauritsen (ANL Staff)
- Marco Siciliano (ANL Staff)

MCS

- Hanqui Guo (ANL/OSU)***
- David Lenz (ANL Pdoc, 25% FOA)
- Sven Leyffer (ANL Staff)
- Thomas Lynn (FOA funded Pdoc)*
- Dominic Yang (UCLA Student)

* Today's Presenters

** On Sabbatical at ANL starting January 2023

*** Transferred to OSU summer of 2022

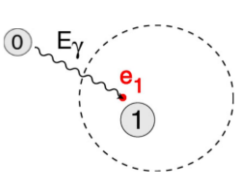
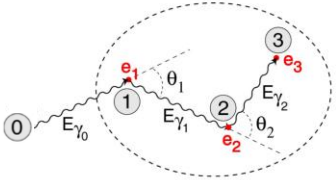
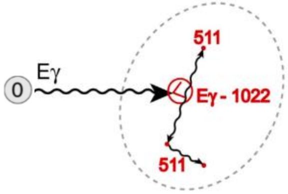
ML TOOLS FOR GAMMA-RAY TRACKING

γ-RAY TRACKING PROBLEM

Overview of the problem

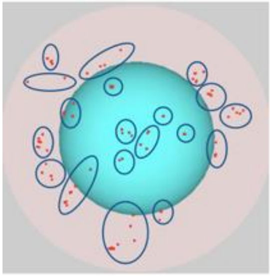
Three interaction types of interest

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

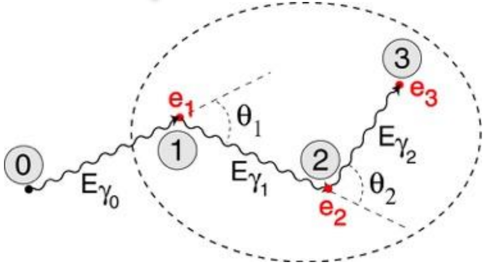
Photoelectric	**Compton Scattering**	**Pair Production**
		
Isolated hits	Angle/Energy	Pattern of hits
Probability of Interaction depth	$E'_{\gamma} = \frac{E_{\gamma}}{1 + \frac{E_{\gamma}}{m_0 c^2}(1 - cos\theta)}$	$E_{1st} = E_{\gamma} - 2m_0c^2$

Three operations

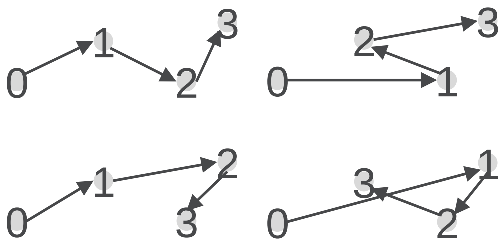
Clustering



Validation



Ordering



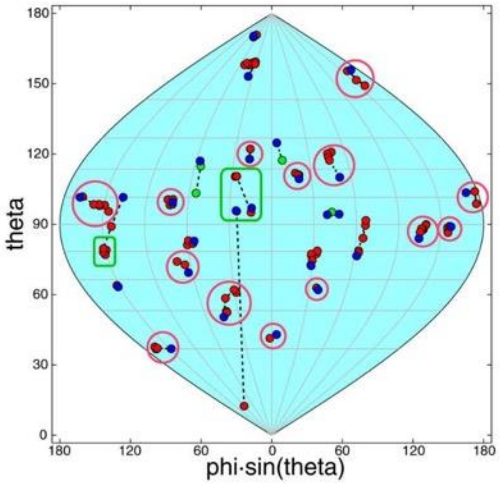
- Doppler correction
- Linear polarization

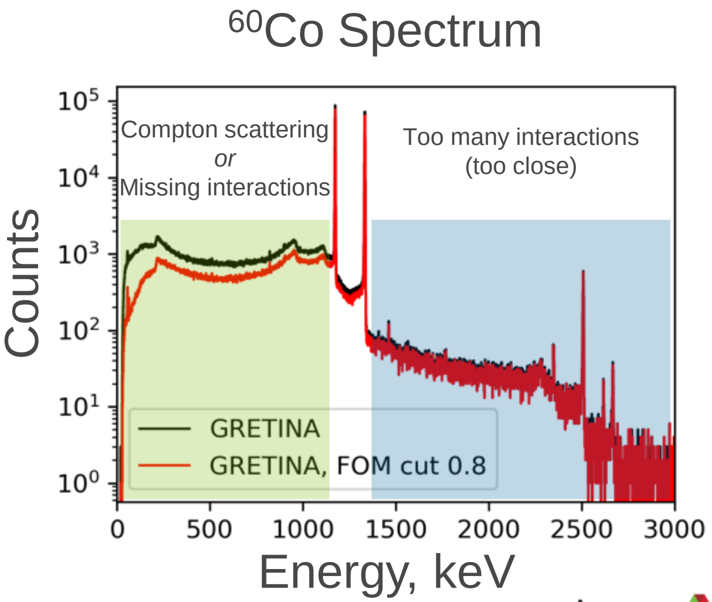
TRACKING PROBLEM: GOALS & CHALLENGES

Using detector information to reconstruct and categorize γ-rays

- Goals:
  1. Find distinct γ-rays (cluster)
  2. Recreate Compton suppression using FOM

- Challenges:
  1. γ-rays too close
  2. γ-ray escape
  3. γ-rays crossing the detector
  4. Suppress environmental γ-rays





ML TOOLS FOR GAMMA-RAY TRACKING

Where ML and data science techniques apply to this problem

Cluster interactions into separate γ-rays

- Energy clustering
- ML clustering
- GNN clustering

Order interactions for individual γ-rays

- Choice of FOM
- Combined clustering/ordering

Suppress γ-rays scattering out of the detector

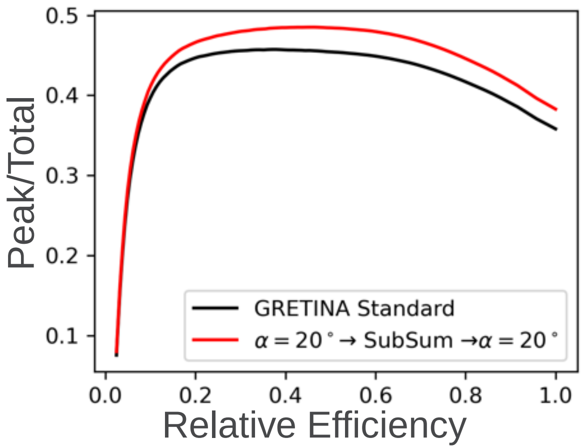
- Choice of FOM
- ML classification
- Recover γ-ray energies

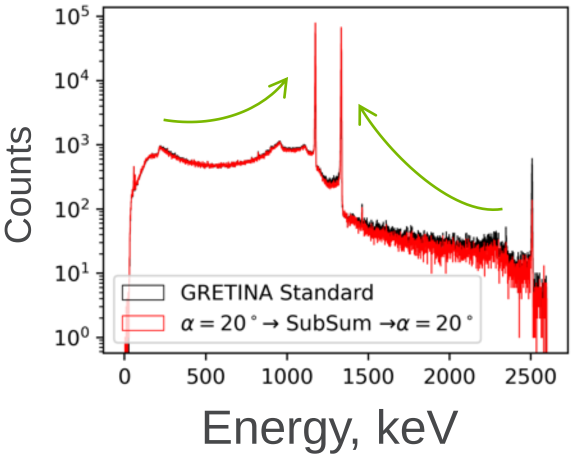
(red text indicates future plans)

ENERGY BASED CLUSTERING

Energy information separates close clusters

- Use spectrum to guide clustering
  – Avoids confusing geometries
- Find interactions with total energy in peaks using a fast MILP solver
- Solve “too big” / “too small” clusters
- Slightly increases P/T and efficiency by capturing more peak energy γ-rays
- Does not create any additional Compton suppression

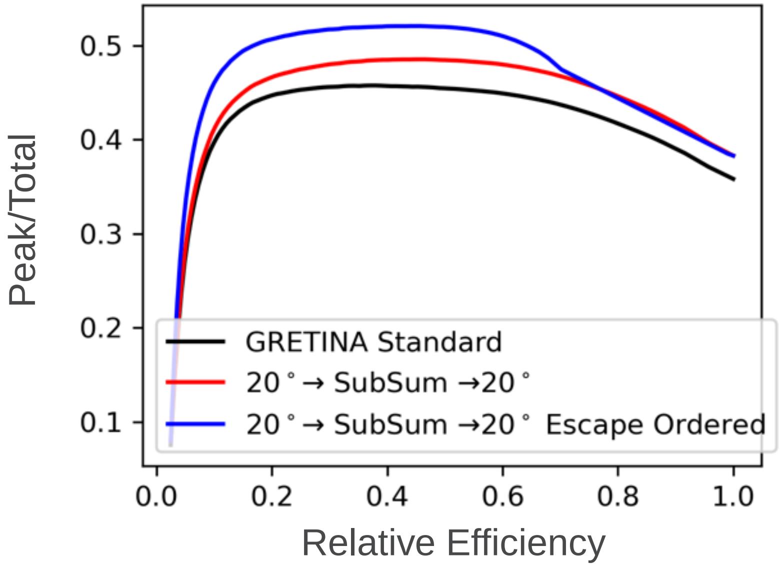




RECREATING COMPTON SUPPRESSION

Correctly ordering escaped γ-rays improves suppression

- Previously done with BGO absorber
- FOM correctly orders < 50% of escapes
  - Wrong order favorable over truth
  - Suppression suffers
- Using escape energy estimate improves suppression (Tashenov & Gerl 2010)
  - Order for escapes is essential for suppression
- ML can further improve ordering & suppression



IMPROVING WITH ML

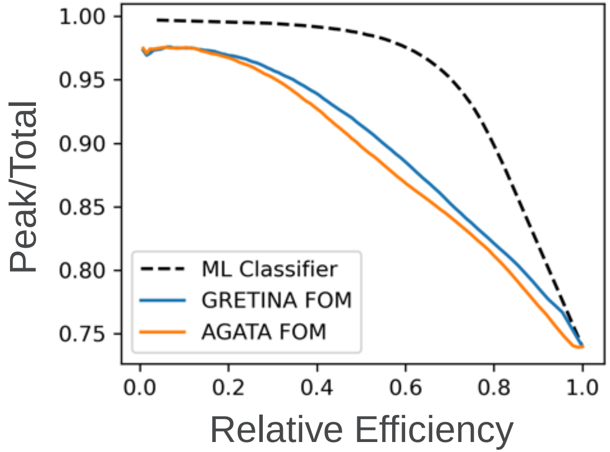
ML tools for ordering & classifying

- Use simulated data:
  - True order is known
  - Escapes are known
- Ordering considerations:
  - Speed, up to $\mathcal{O}(n!)$
  - Absolute FOM value is not important, only relative
- ML Escape classification
  - Assume clustered
- Challenging to transfer model to experimental data

Ordering Consistency

Multiplicity 30 data	GRETINA FOM	GRETINA Escape	AGATA FOM	ML FOM
Complete γ	73.8%	73.4%	87.0%	81.4%
Escape γ	46.7%	58.0%	76.2%	77.5%
Total	67.0%	69.5%	85.2%	80.4%

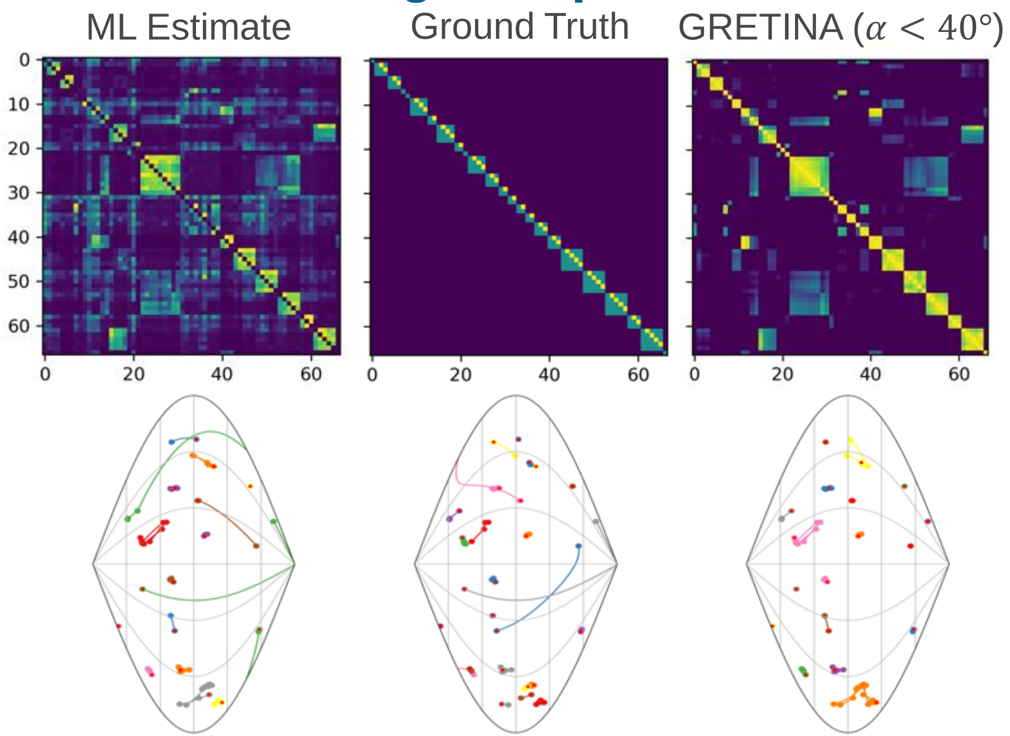
Without single interactions



ML CLUSTERING

Clustering beyond GRETINA without knowledge of spectrum

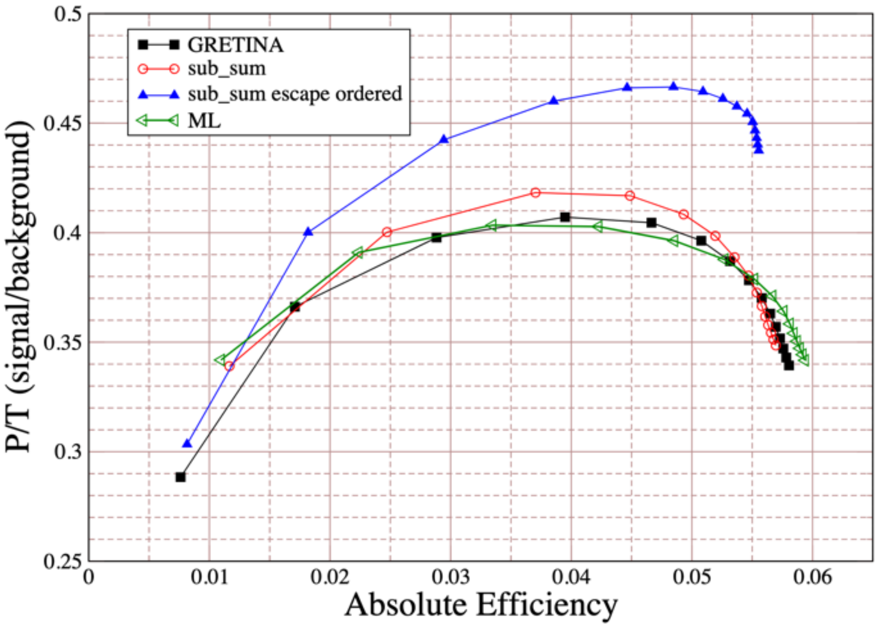
- GRETINA clustering is done spatially with respect to cluster spread (scattering forward)
- Use ML to create an alternate distance metric by which to cluster
  - Learned from data
  - Include additional clustering steps beyond singles
  - Include cluster order



FUTURE WORK AND EXTENSIONS

Improving the resolving power of GRETINA for further analysis

- Improved recovery of escape energies instead of suppression
- ML tools for fast tracking
- ML training using experimental data from sources
- ML tools for on-line learning
- Optimization based approaches for better clustering
- Apply techniques to the problem of pair production

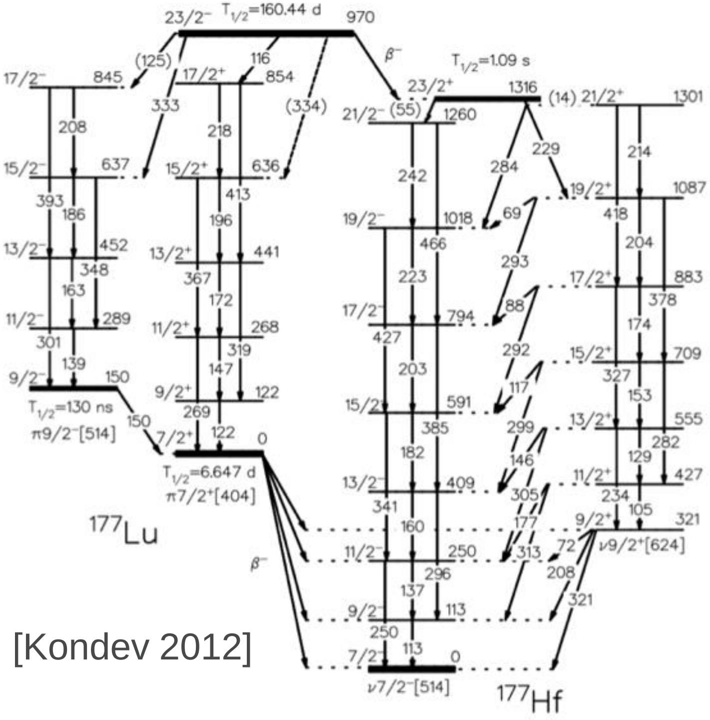


ML TOOLS FOR LEVEL-SCHEME DESIGN

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

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:

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

ML TOOLS FOR LEVEL-SCHEME DESIGN

Inverse Optimization to Determine Transitions

- Goal: Given *S*, *C*, find *A*, *D* such that

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

- Formulate nonlinear constrained optimization problem:

$$\begin{aligned} \underset{A,D}{\text{minimize}} \quad & \| D - S\left((I-A)^{-1} - I\right) \|^2_{\Gamma^{-1}} + \text{prior}(A) \\ \text{subject to} \quad & \boxed{A \geq 0, \sum_j A_{ij} \leq 1}, \; C = D + D^T \end{aligned}$$

$$\boxed{\begin{aligned} \underset{A,D,T}{\text{minimize}} \quad & \| D - ST \|^2_{\Gamma^{-1}} + \text{prior}(A) \\ \text{subject to} \quad & (I - A)(T + I) = I \\ & \boxed{A \geq 0, \sum_j A_{ij} \leq 1}, \; C = D + D^T. \end{aligned}}$$

Enforce constraints such as conservation of energy, nonnegative decay intensities etc

ML TOOLS FOR LEVEL-SCHEME DESIGN

Optimization Techniques

- Inverse optimization for transitions *A*
- Use nonlinear optimization methods
  … solves within minutes on laptop
- Extends to γ-γ-γ-interactions (tensors)

$$\begin{aligned} \underset{A,D,T}{\text{minimize}} \quad & \|D - ST\|^2_{\Gamma^{-1}} + \text{prior}(A) \\ \text{subject to} \quad & (I - A)(T + I) = I \\ & A \geq 0, \ \sum_j A_{ij} \leq 1, \ C = D + D^T. \end{aligned}$$

- **<u>Progress so Far</u>:**
  - Implemented inverse optimization in AMPL & solve model using IPOPT
  - Successful proof-of-concept:
    (1) Generate data *(S,C)* from given level-scheme (python code)
    (2) Solve inverse optimization for *A* (AMPL/IPOPT)
    (3) Create level-scheme & compare to original scheme

LEVEL SCHEME RECONSTRUCTION

Actionable Physics from Output Matrices

- Inverse optimization results in two matrices:
  - *A:* the matrix of branching ratios between subsequent γ-rays
  - *D*: the <u>directed</u> coincidence data

- Final Step: Create energy level scheme from matrix output

```
[[   0.      0.      0.      0.      0.      0.      0.      0.      0.      0.  ]
 [4068.      0.      0.      0.      0.      0.      0.      0.      0.      0.  ]
 [   0.      0.      0.      0.      0.      0.      0.      0.      0.      0.  ]
 [3563.05 3563.05 4809.95    0.      0.      0.      0.      0.      0.      0.  ]
 [   0.      0.      0.      0.      0.      0.      0.      0.      0.      0.  ]
 [4229.02 4229.02 5708.98    0.      0.      0.      0.      0.      0.      0.  ]
 [   0.      0.      0.      0.      0.      0.      0.      0.      0.      0.  ]
 [1731.1  1731.1  2336.9  4068.      0.      0.      0.      0.      0.      0.  ]
 [1486.44 1486.44 2006.62    0.   4097.94 3493.06    0.      0.      0.      0.  ]
 [   0.      0.      0.      0.      0.      0.      0.      0.      0.      0.  ]]
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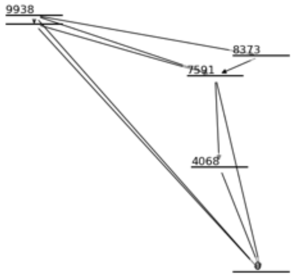


ML TOOLS FOR LEVEL-SCHEME DESIGN

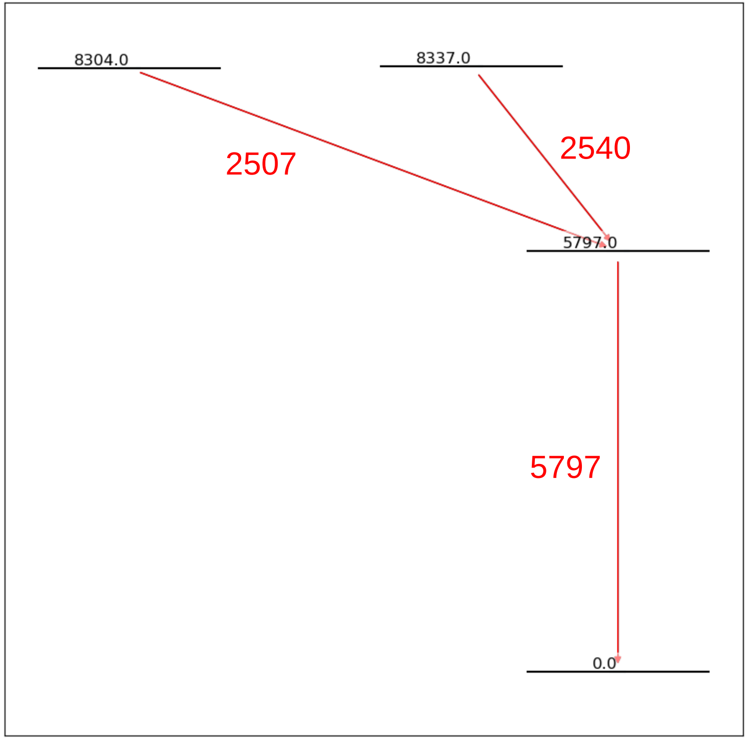
Level-Scheme Representation from Transition Matrix

Outgoing gamma energy

Incoming gamma energy

Weighted Adjacency =

	2507	2540	4117	4150	4187	4945	5797	8337	9094	13282
2507	0	0	0	0	0	0	228	0	0	0
2540	0	0	0	0	0	0	1767	0	0	0
4117	0	0	0	0	546	0	0	0	0	0
4150	0	0	0	0	565	0	0	0	0	0
4187	0	0	0	0	0	0	0	0	0	0
4945	0	134	0	43	0	0	0	14	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	298	0	0	0	0	0
13282	0	0	0	0	0	0	0	0	0	0



ML TOOLS FOR LEVEL-SCHEME DESIGN

Level-Scheme Representation from Transition Matrix

Weighted Adjacency =

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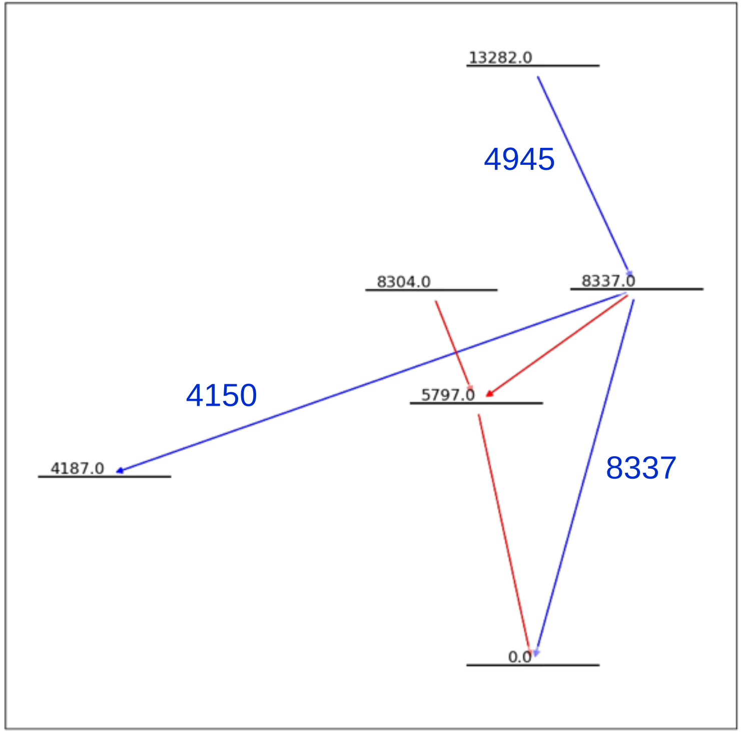
9094	0	0	0	0	298	0	0	0	0	0
13282	0	0	0	0	0	0	0	0	0	0

*Adjacent transition



ML TOOLS FOR LEVEL-SCHEME DESIGN

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4945	0	134	0	43	0	0	0	14	0	0
5797	0	0	0	0	0	0	0	0	0	0
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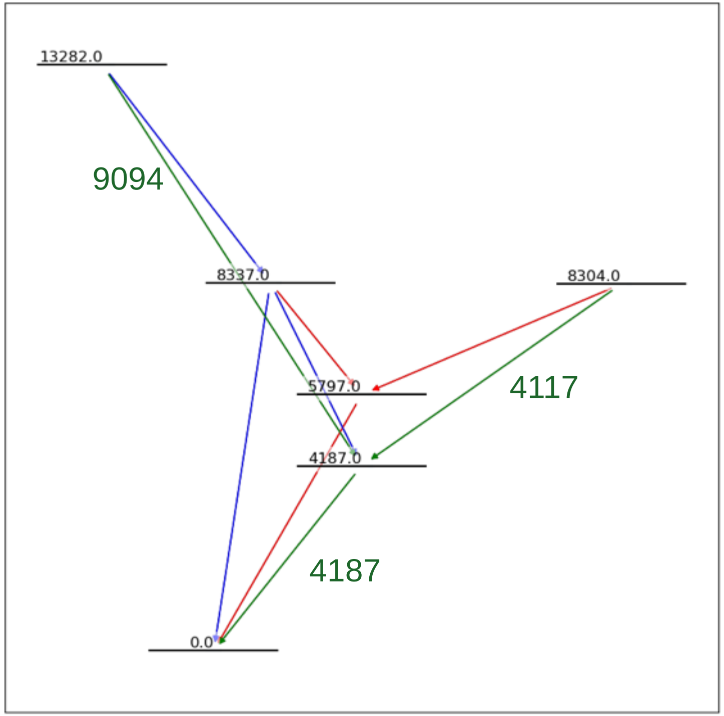
*Adjacent transition



FUTURE WORK AND EXTENSIONS

- Develop tools to automatically extract γ-ray intensity information for 2- and 3-fold coincidence data.
- Handling of uncertainty/noise with level-scheme construction for robust results
- Level scheme from γ-γ-γ interactions
- Fast ML-inspired algorithms (ADMM) for level-scheme construction
- Apply algorithms to both simulated data and experimental data where gamma-ray intensities have been extracted with developed tools.

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	310 (FY22)	40 (FY23)	350

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

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