Machine Learning for the Automated Analysis of Data from Large-Scale Gamma-Ray Spectrometers

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Presentation Outline

1

Gamma-Ray Data Challenges

Large-scale gamma-ray data requires advanced analysis. Traditional methods struggle with volume and complexity.

2

Machine Learning Approach

We apply ML algorithms for automated interpretation.

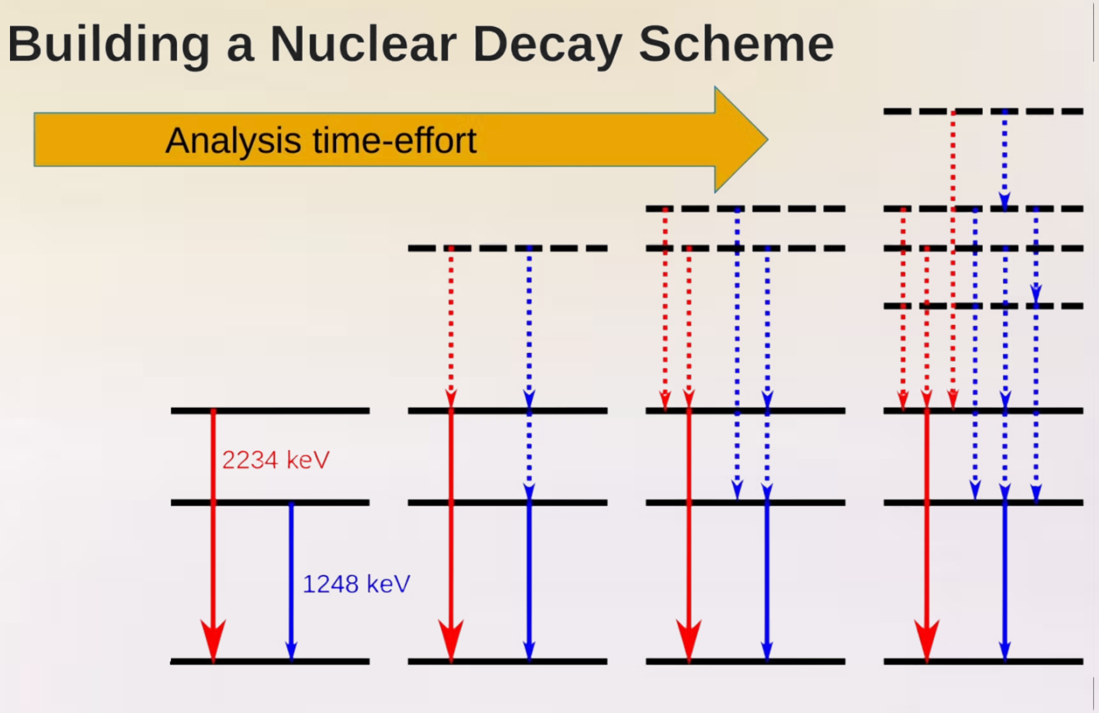
3

Impact and Future Prospects

ML enhances accuracy and speed. It offers new insights for scientific discovery and applications.

Why Building Level Schemes Still Hurts

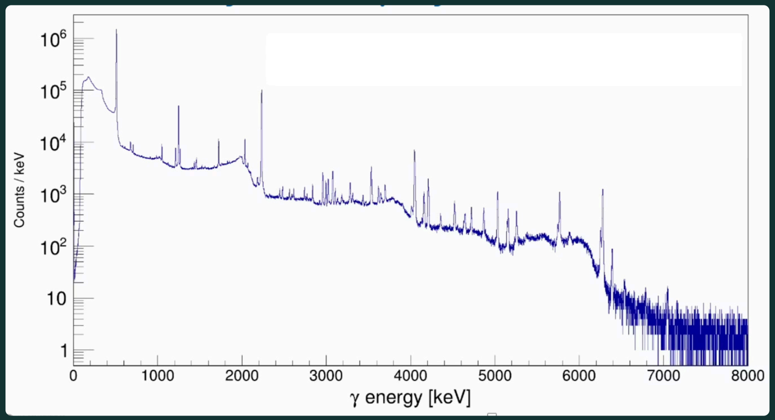
Manually building level schemes from gamma-ray data is immensely complex. It demands significant expertise and time, often struggling with vast, intricate datasets.



The Data: Singles Matrix and Gamma-Gamma Coincidence Matrix

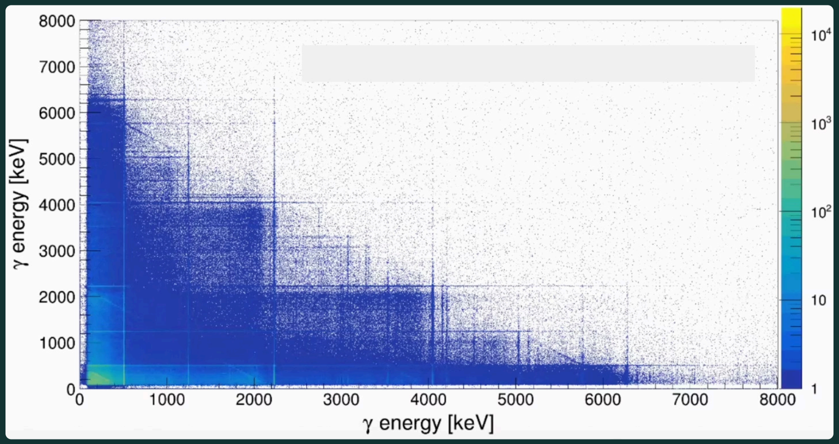
Understanding raw gamma-ray measurements is essential. We analyze both individual energy events and correlated detections. These matrices form the foundation for our automated analysis.

Singles Matrix



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

Gamma-Gamma Coincidence Matrix

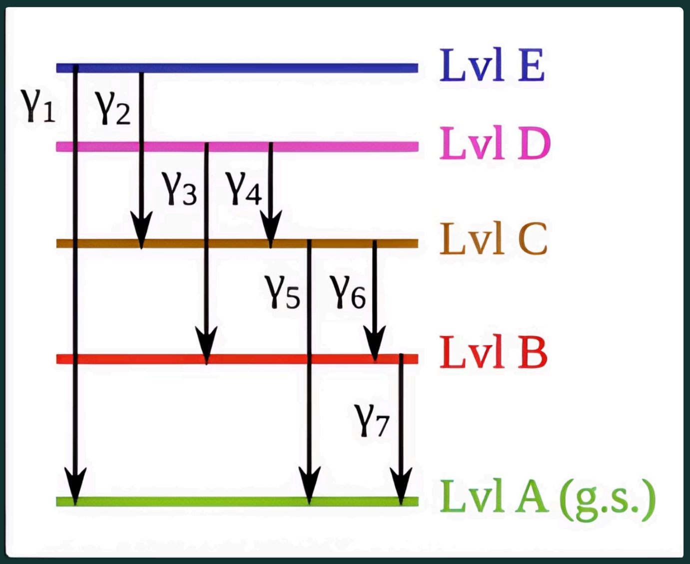


$$C = \begin{pmatrix} C_{11} & C_{12} & \cdots & C_{1n} \\ C_{21} & C_{22} & \cdots & C_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ C_{n1} & C_{n2} & \cdots & C_{nn} \end{pmatrix}$$

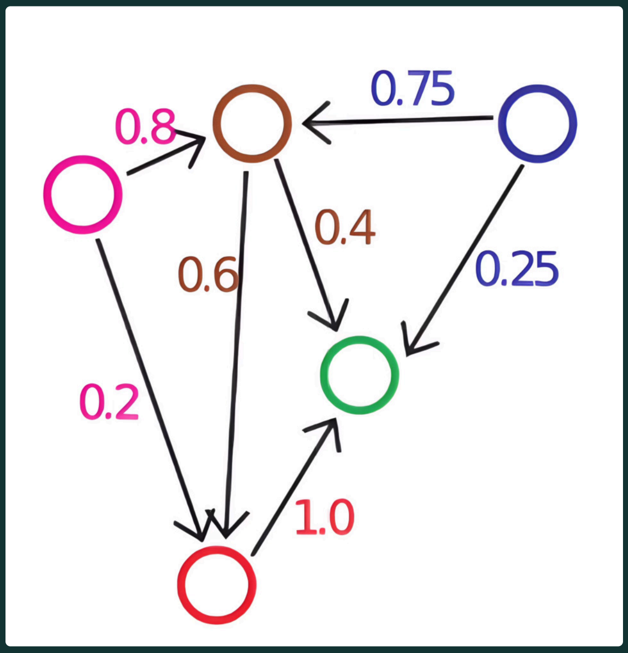
Data Representation as Graph

- Gamma-ray data can be represented as a mathematical graph structure. This enables powerful computational approaches for level scheme reconstruction.

Decay Scheme

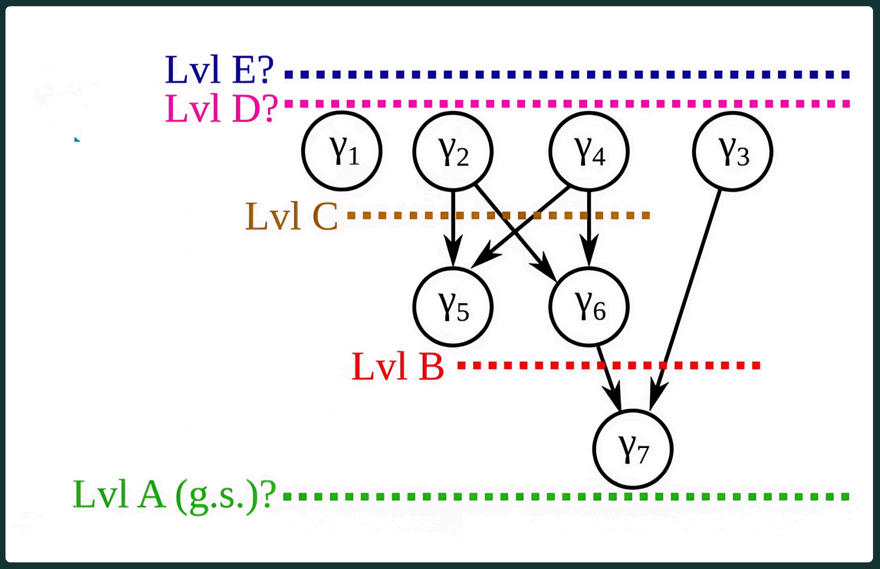


Level Centric Graph



- 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

Transition Centric Graph



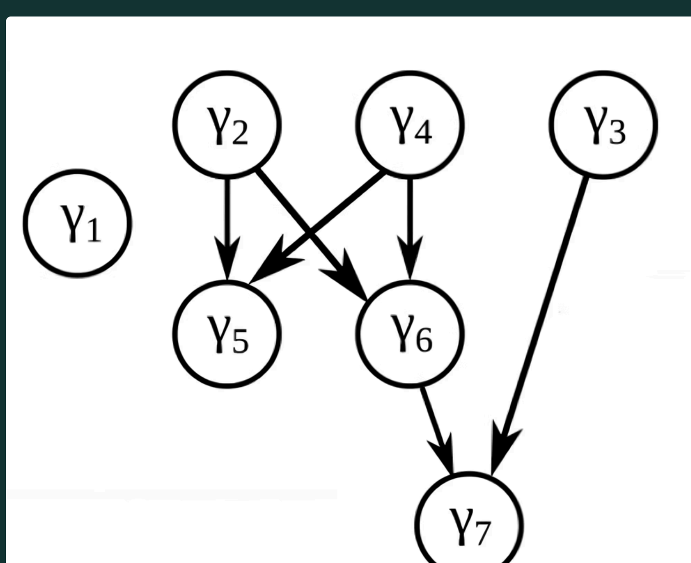
- In this representation, vertices correspond to observable γ-rays, while edges connect gamma-ray transitions detected in coincidence
- A unique transition centric graph exists for every level-centric decay scheme, but additional information required to reconstruct level-centric decay schemes from transition-centric graph

Data Representation as Graph

Adjacency Matrix

Gamma-ray data can be represented as a mathematical graph structure. This enables powerful computational approaches for level scheme reconstruction.

- Every weighted, directed graph has a unique adjacency matrix A
- Given a start position of vertex i, element Aij is the probability of transitioning directly to vertex j (non-zero numbers = branching ratios)



$$A = \left(\begin{array}{c|ccccccc} & \gamma_1 & \gamma_2 & \gamma_3 & \gamma_4 & \gamma_5 & \gamma_6 & \gamma_7 \\ \hline \gamma_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \gamma_2 & 0 & 0 & 0 & 0 & 0.4 & 0.6 & 0 \\ \gamma_3 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0 \\ \gamma_4 & 0 & 0 & 0 & 0 & 0.4 & 0.6 & 0 \\ \gamma_5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \gamma_6 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0 \\ \gamma_7 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{array}\right)$$

Evolutionary - Optimization Algorithm

Numerical Solution:

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

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

- Therefore we have two governing equations:

$$\begin{aligned} D &= S\left((I - A)^{-1} - I\right) \\ C &= D + D^T \end{aligned}$$

- Satisfying both equations leads to the nonlinear optimization problem:

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

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

G. A. Demand, **"Development of a Novel Algorithm for Nuclear Level Scheme Determination."** M.Sc. thesis, Department of Physics, University of Guelph, 2009. Available at https://hdl.handle.net/10214/20603.

Machine Learning Tools for Level-Scheme Design:

Learn the Guess - Keep the Physics

This approach automates scheme design. It learns to propose. It keeps physical laws.

Automate Initial Hypotheses

ML identifies patterns. It proposes initial schemes. This reduces manual effort.

Preserve Physical Principles

The system validates suggestions. It adheres to physics laws. Accuracy is maintained.

Machine Learning Architecture

1 Vision Tranformer (ViT) Encoder

- Take the 2D coincidence matrix "C" and singles vector "S", chop C into patches, and run them (with a learned CLS token) through a stack of self-attention layers to produce a single global embedding that captures all the correlations in the data.

2 AutoRegressive Decoder

- Conditioned on that CLS embedding (and the singles-spectrum embedding), unroll one token at a time—first the gamma-ordering, then the branching fractions—so as to generate a fully-specified candidate level-scheme (i.e. the A - matrix)

3 Warm Start Deterministic Polish

- Seed a light - weight evolution/hill-climb solver with the network's guess and run a few dozen generations of small perturbations—enforcing hard physics constraints (energy conservation, non-negative intensities, correct gap equations)—to converge on a physically consistent final solution.

SurrogateNet Architecture

(C,S) —— ▶️ Encoder —— ▶️ h —— ▶️ Decoder —— ▶️ token stream —— ▶️ Row Softmax —— ▶️ Â

1

Vision Tranformer (ViT) Encoder

2

AutoRegressive Decoder

(C, S)

- **C** is your 2D γ–γ coincidence matrix (counts of "γ i coincident with γ j"), shaped [n,n]
- **S** is your 1D singles spectrum (total counts per γ), shaped [n]

▶️ Encoder

- A Vision - Transformer takes C (as a little "image" of size n×n, chopped into patches) and S (via a small MLP)
- It runs them through self - attention layers, producing a **single embedding vector** h that summarizes all of C + S.

▶️ h

- Latent **summary** (CLS token output of the ViT)
- Carries all the learned information about which coincidences and singles patterns are in the input.

▶️ Decoder

- An autoregressive module that "unrolls" h into a sequence of outputs (the "token stream").

▶️ token stream

- The raw logits or token indices that represent:
  - **which γ comes from which level** (ordering tokens)
  - **how much of each γ's intensity branches to each sibling** (branching - fraction tokens)

▶️ Row-softmax

- Reshape that vector to an $n \times n$ matrix
- Clamp negatives → apply softmax **row-by-row**
- Ensures non-negativity & each row sums to 1

▶️ Â

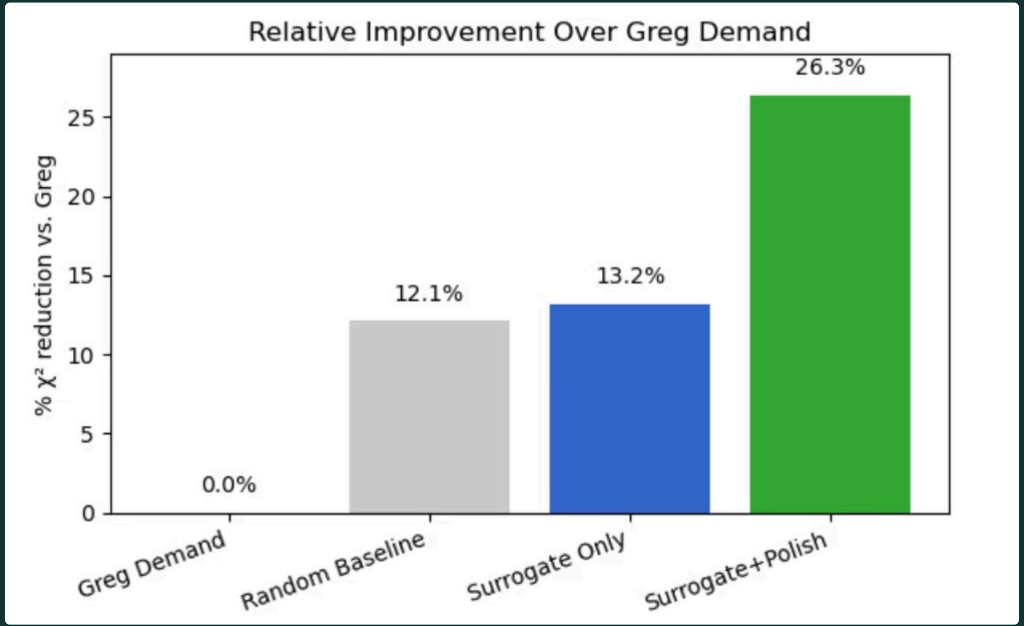
- The final **predicted A-matrix** of branching ratios, ready for loss calculation (supervised MSE vs. true A, and physics χ^2 vs. C_exp).

Proof of Concept

Synthetic Engine:

Tested on synthetic gamma-ray spectrometer data. Initial results confirm its efficacy. This paves the way for advanced automation.

Our proof of concept validates the SurrogateNet architecture. It demonstrates the system's ability to automate level scheme analysis.



Future Work & Next Steps

Why it matters

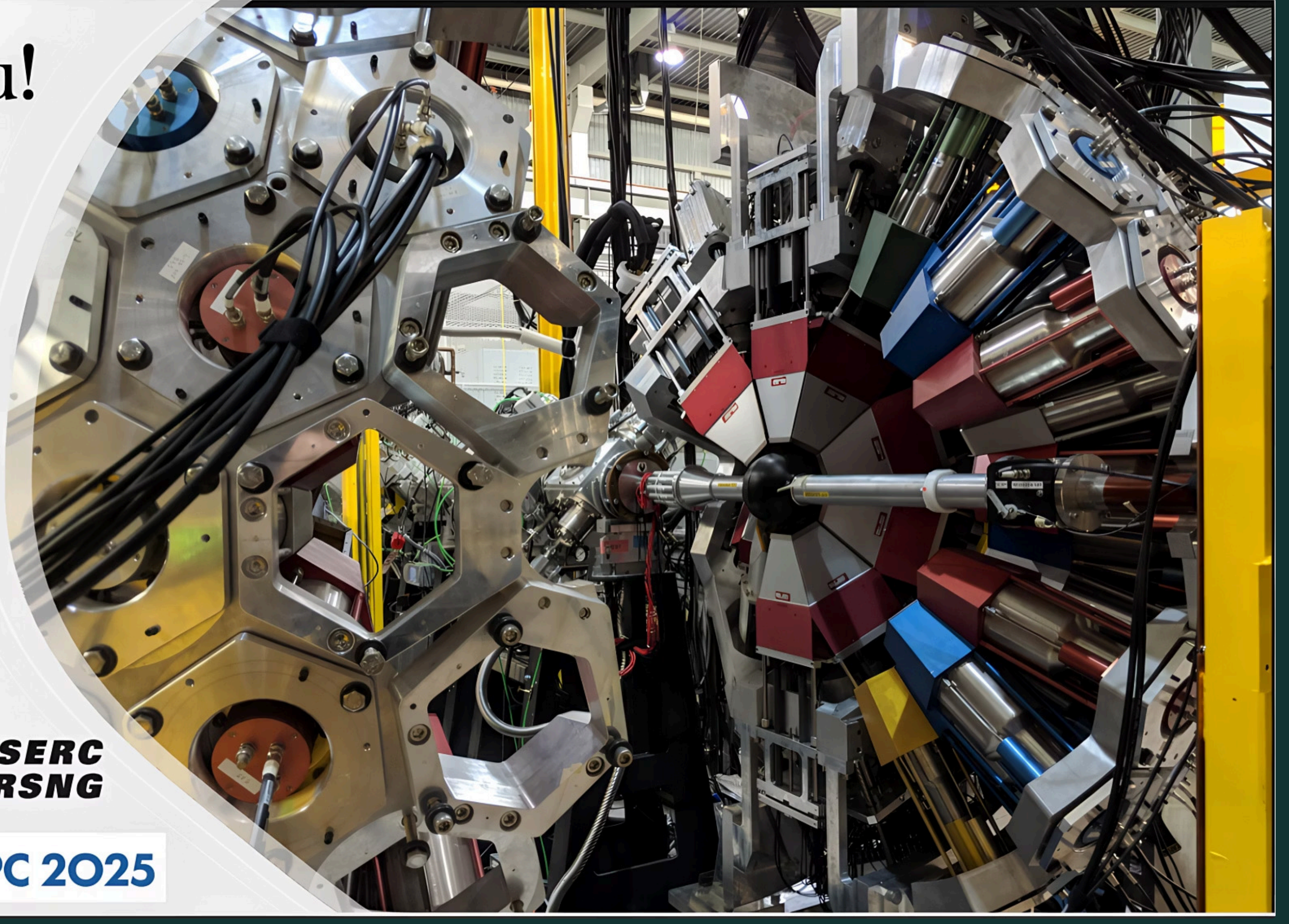
- The **encoder** (Vision Transformer) learns **global γ–γ context**—vital for spotting which peaks correlate.
- The **decoder** generates **variable-length** level schemes, enforcing row sums by design.
- **Supervised training** on realistic synthetic data teaches the network to make a **very good first guess**, offering potential orders of magnitude speed up.

Next

- Scale up the surrogate model and run on real experimental data (S and C's).
- Need auxiliary tools to optimize the S and C's that are fed into the SurrogateNet process; think peak detection, background subtraction, doublet resolution, etc.
- Develop user-friendly interfaces for physicists. Streamline the automated level scheme design process.

> This will not steal your job !
>
> 😄

Thank you!



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